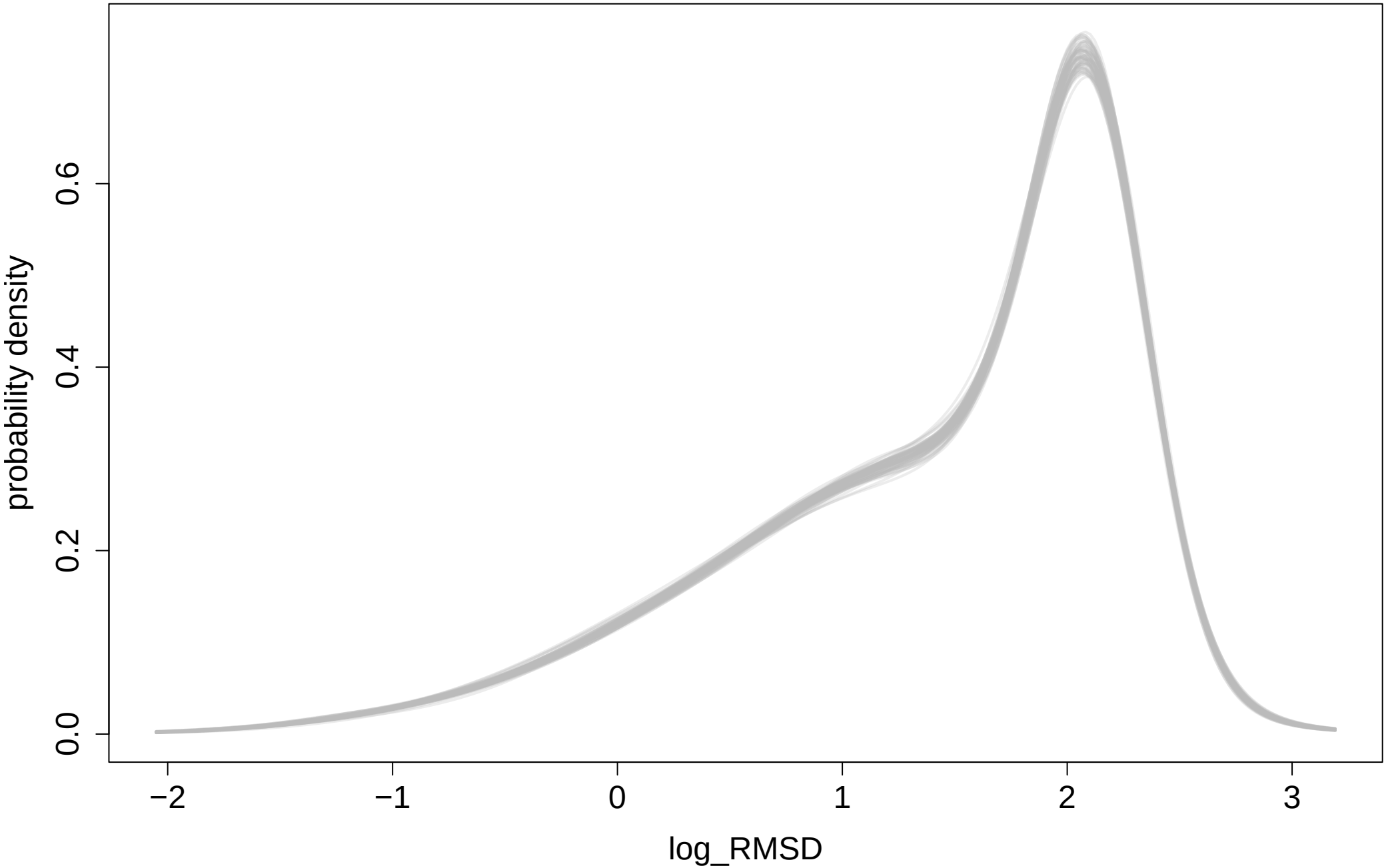
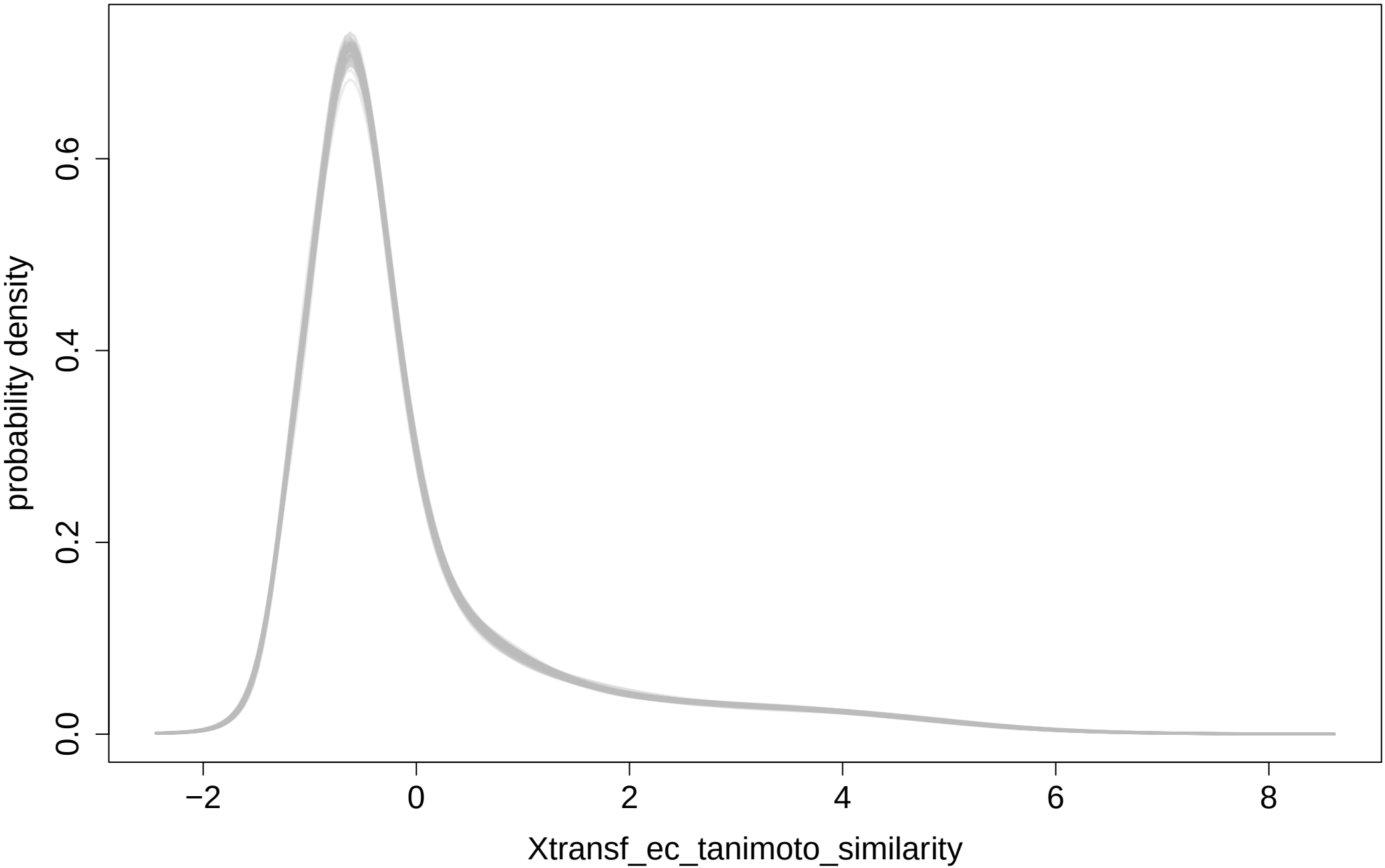
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.118861696140895
max MCSE = 8.83527183026341
all stationary: FALSE
burn: 0

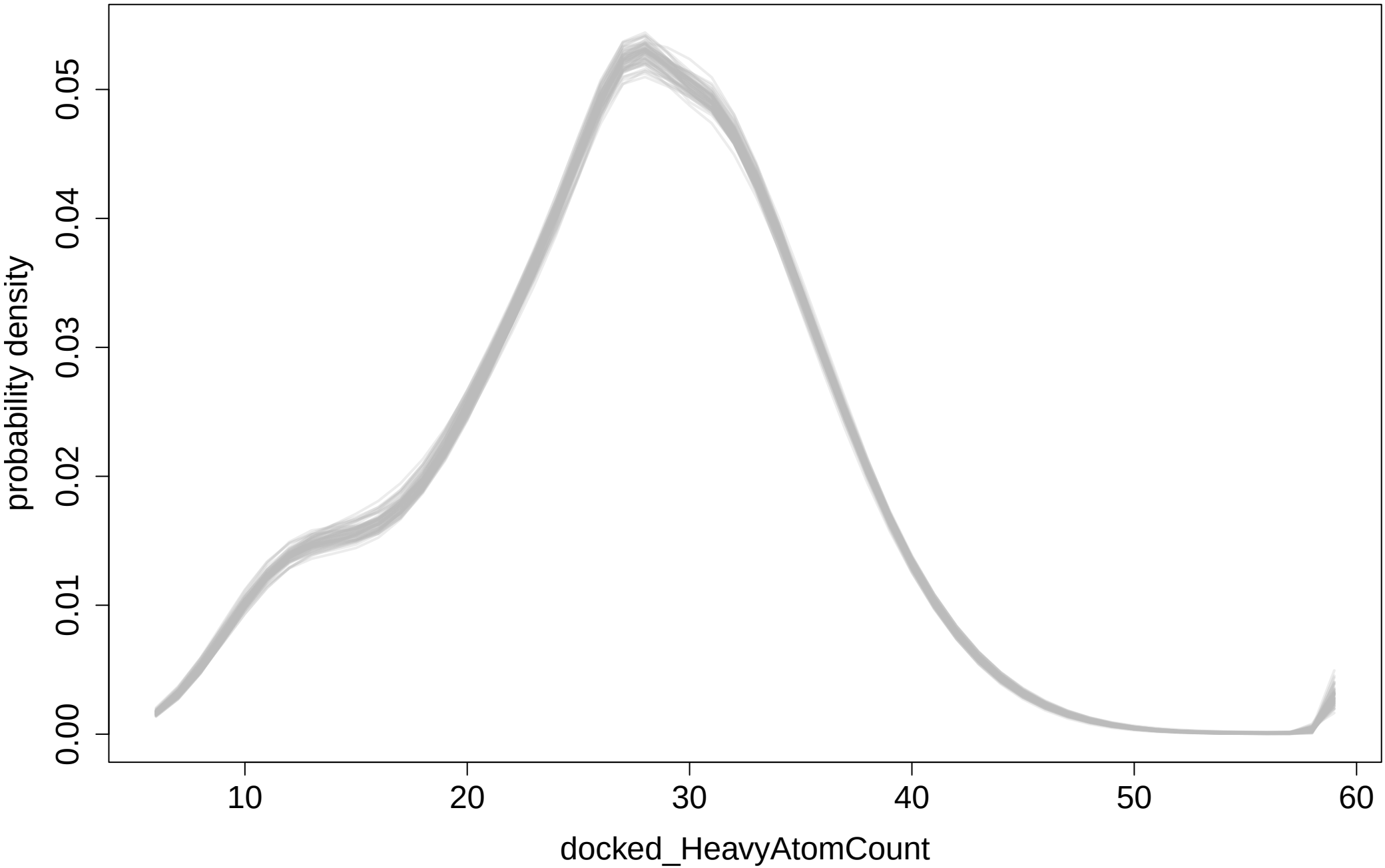
−− STATS 2D −−
min ESS = 1590.77829959805
max BMK = 0.059146041832711 7
max MCSE = 2.78073046797518
all stationary: FALSE
burn: 0

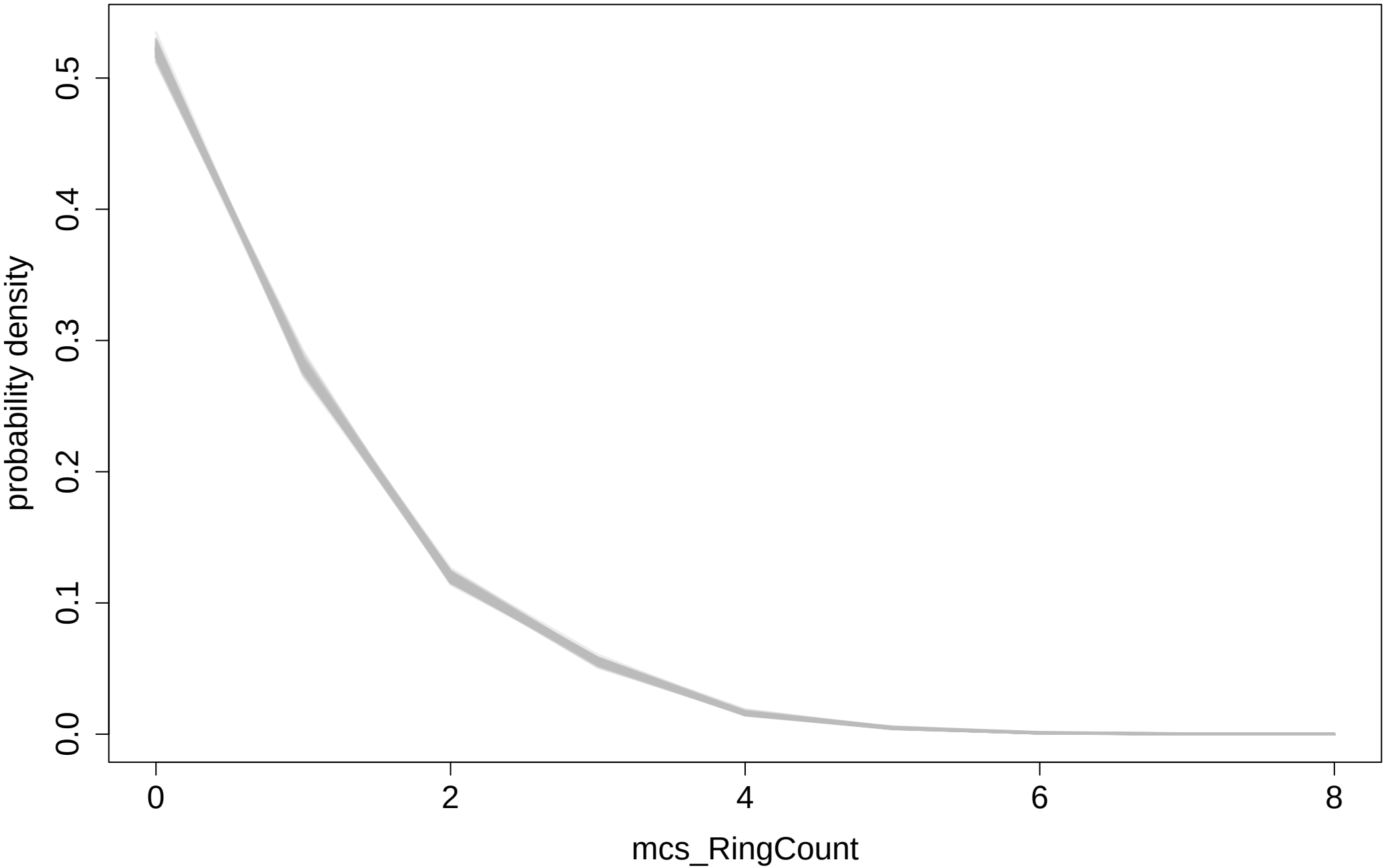
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = NaN
all stationary: FALSE
burn: 2040

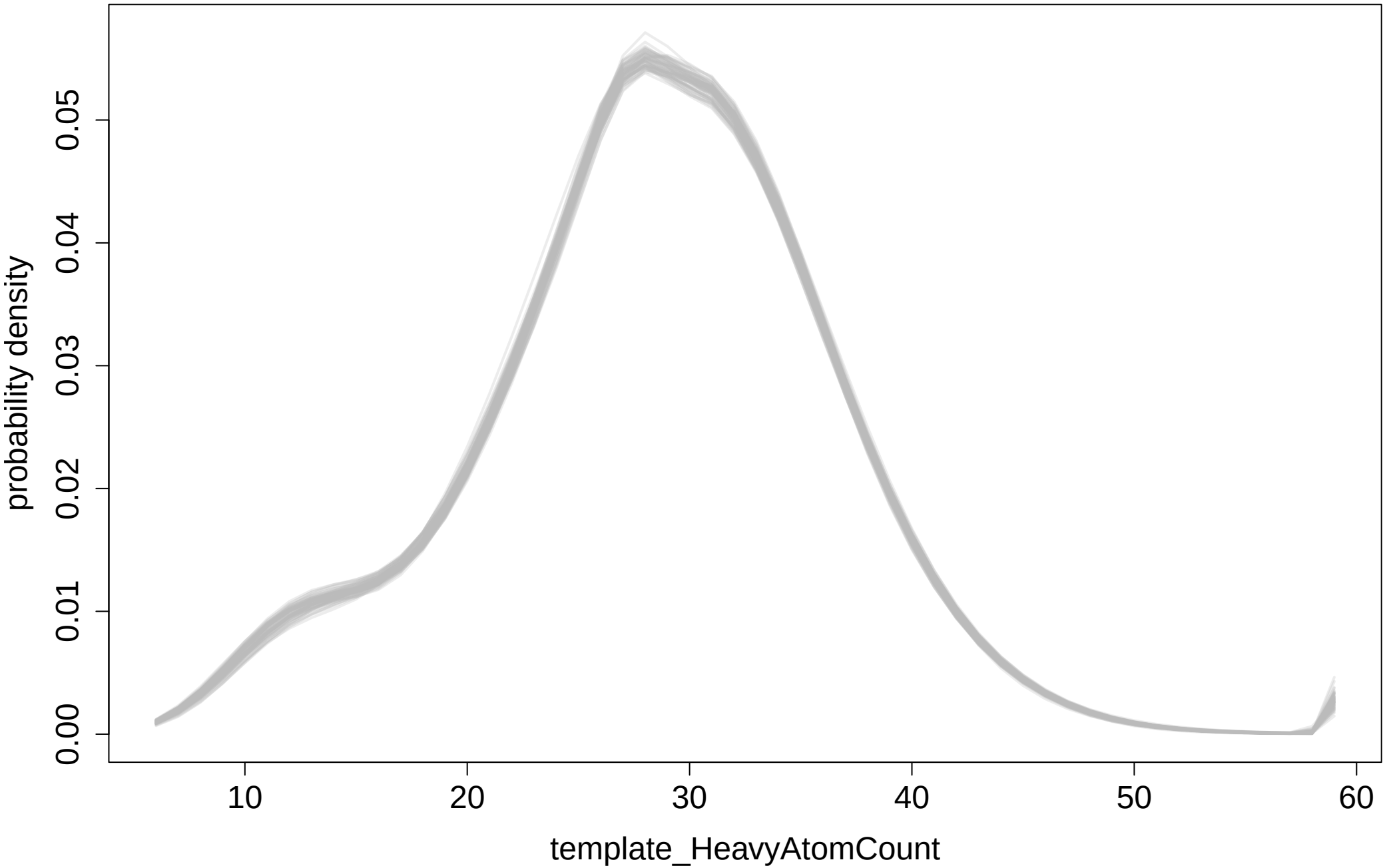
Occupied clusters: 62 of 64
LL: −110000 +− 24.5

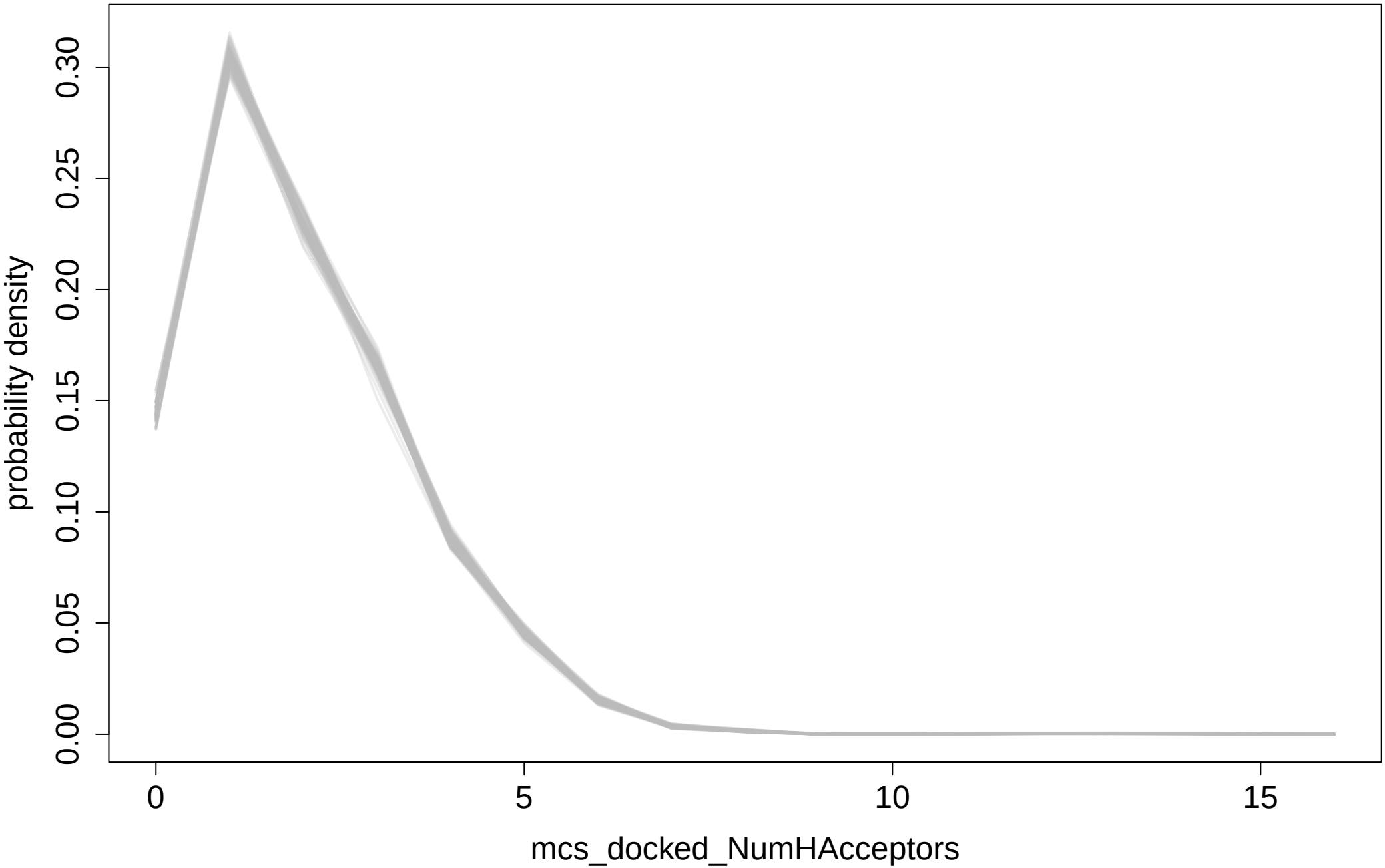

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

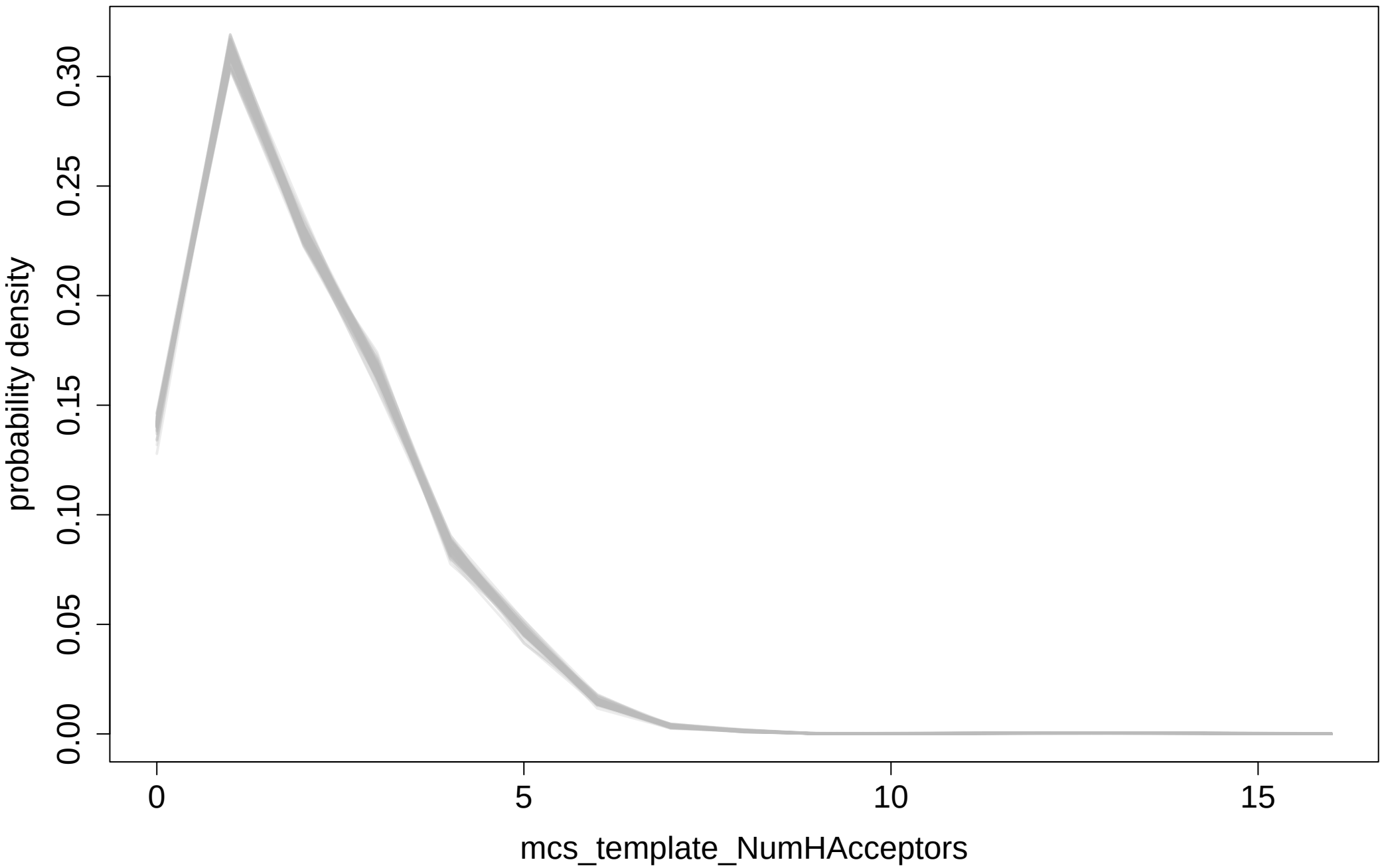

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

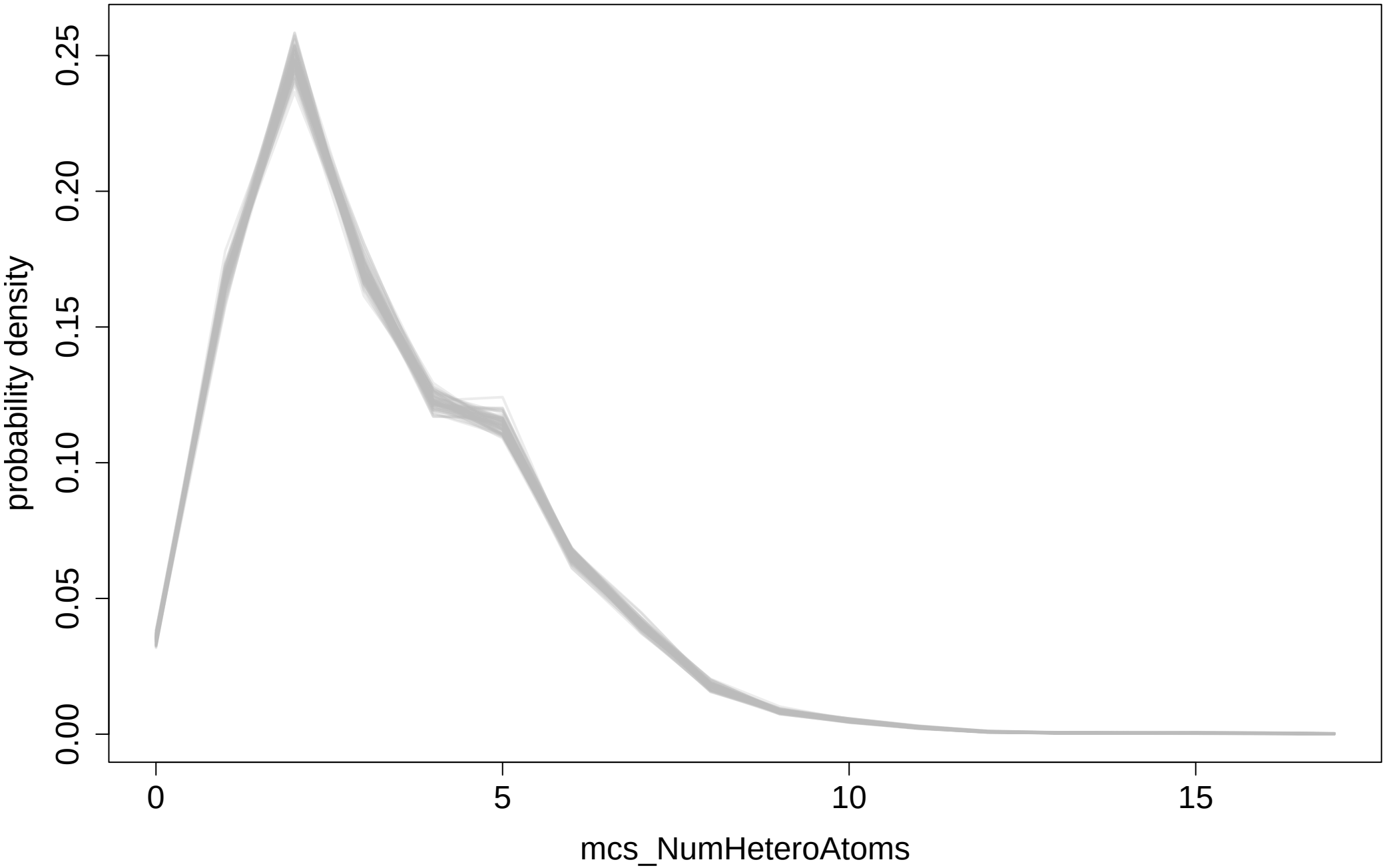

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

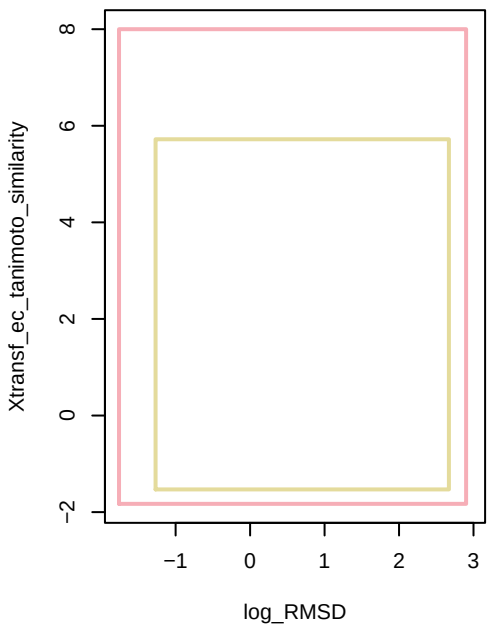

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

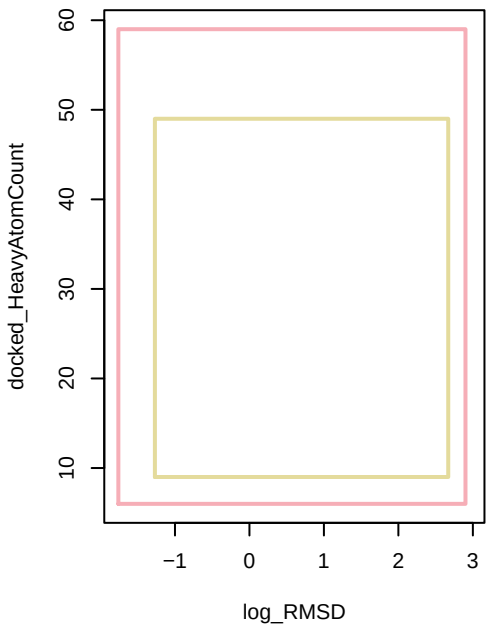

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

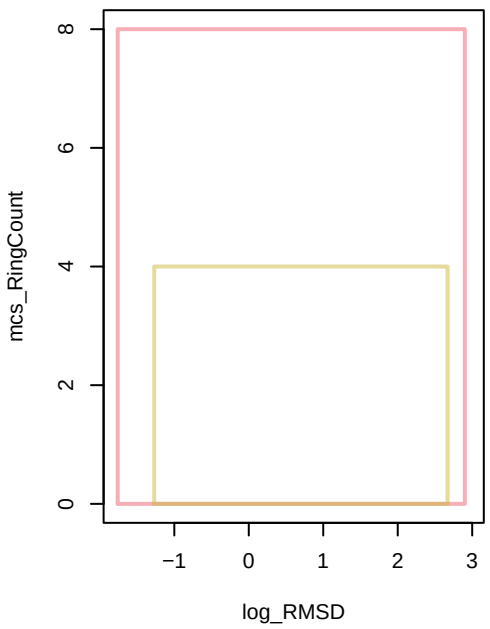

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

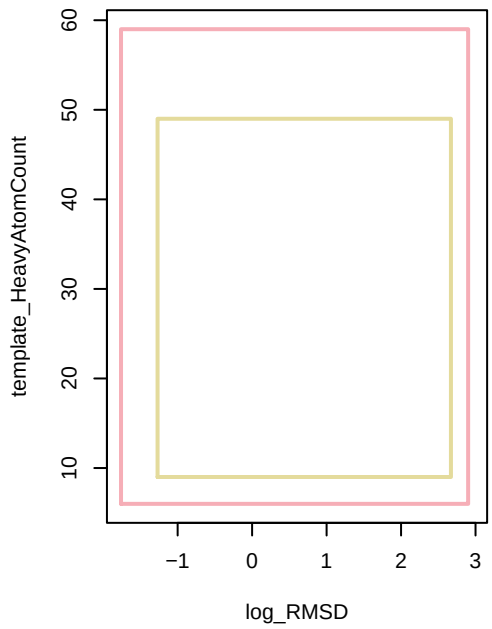

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

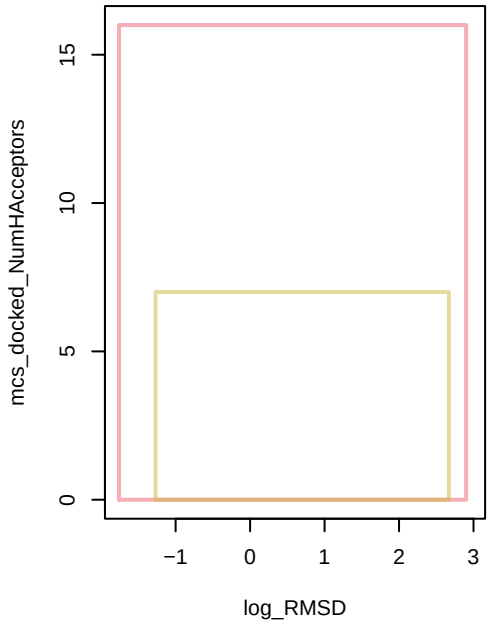

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

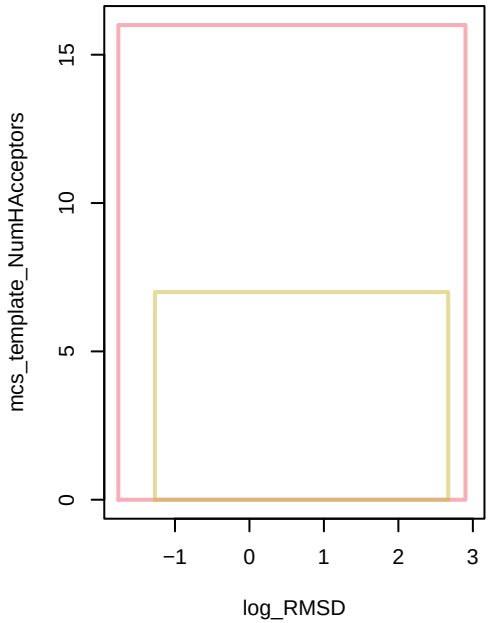

Xtransf_ec_tanimoto_similarity
log_RMSD

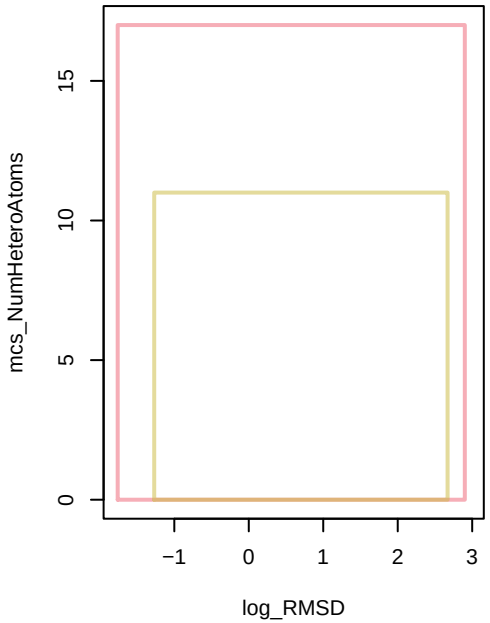

docked_HeavyAtomCount
log_RMSD

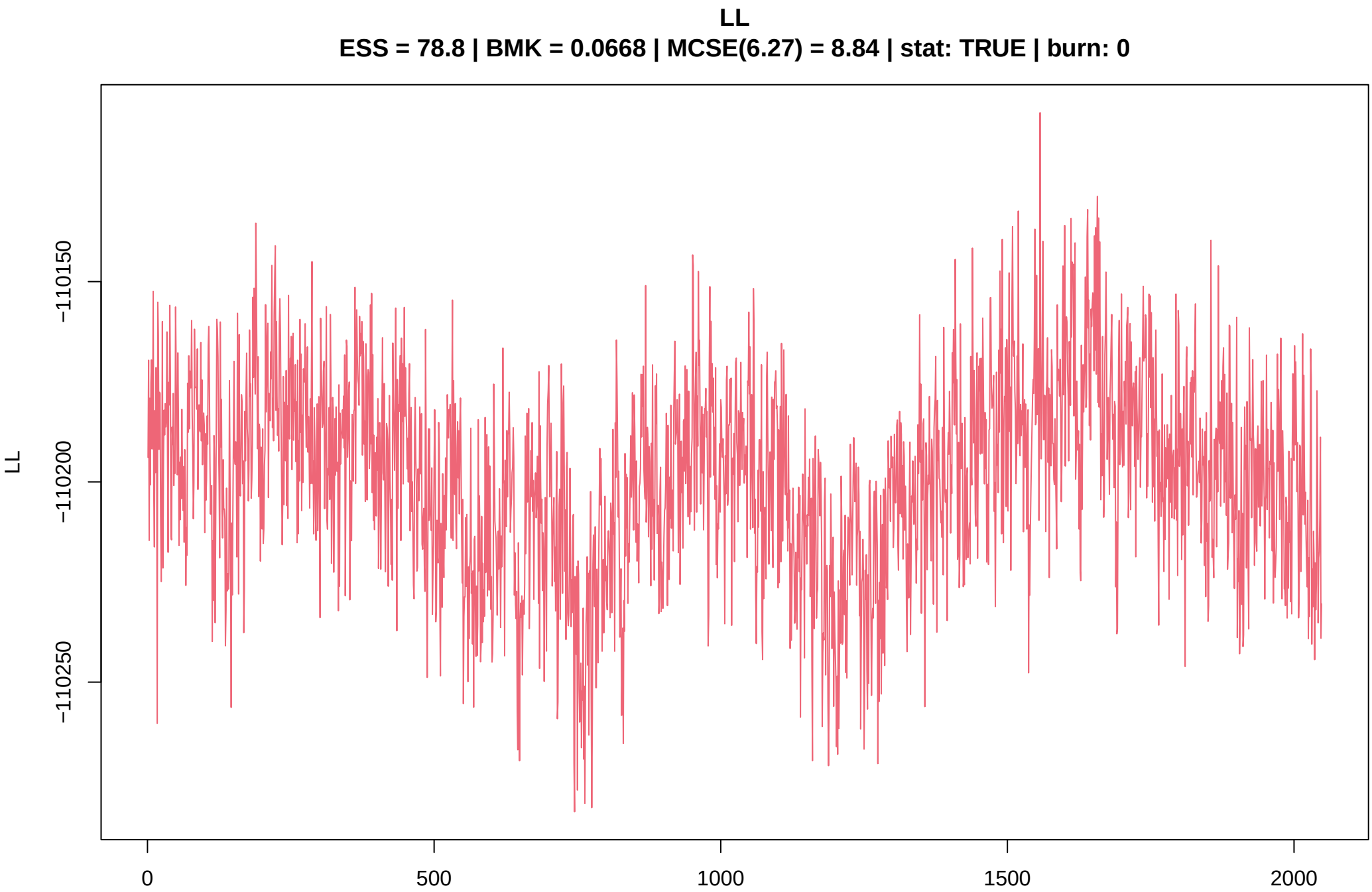

mcs_RingCount
log_RMSD

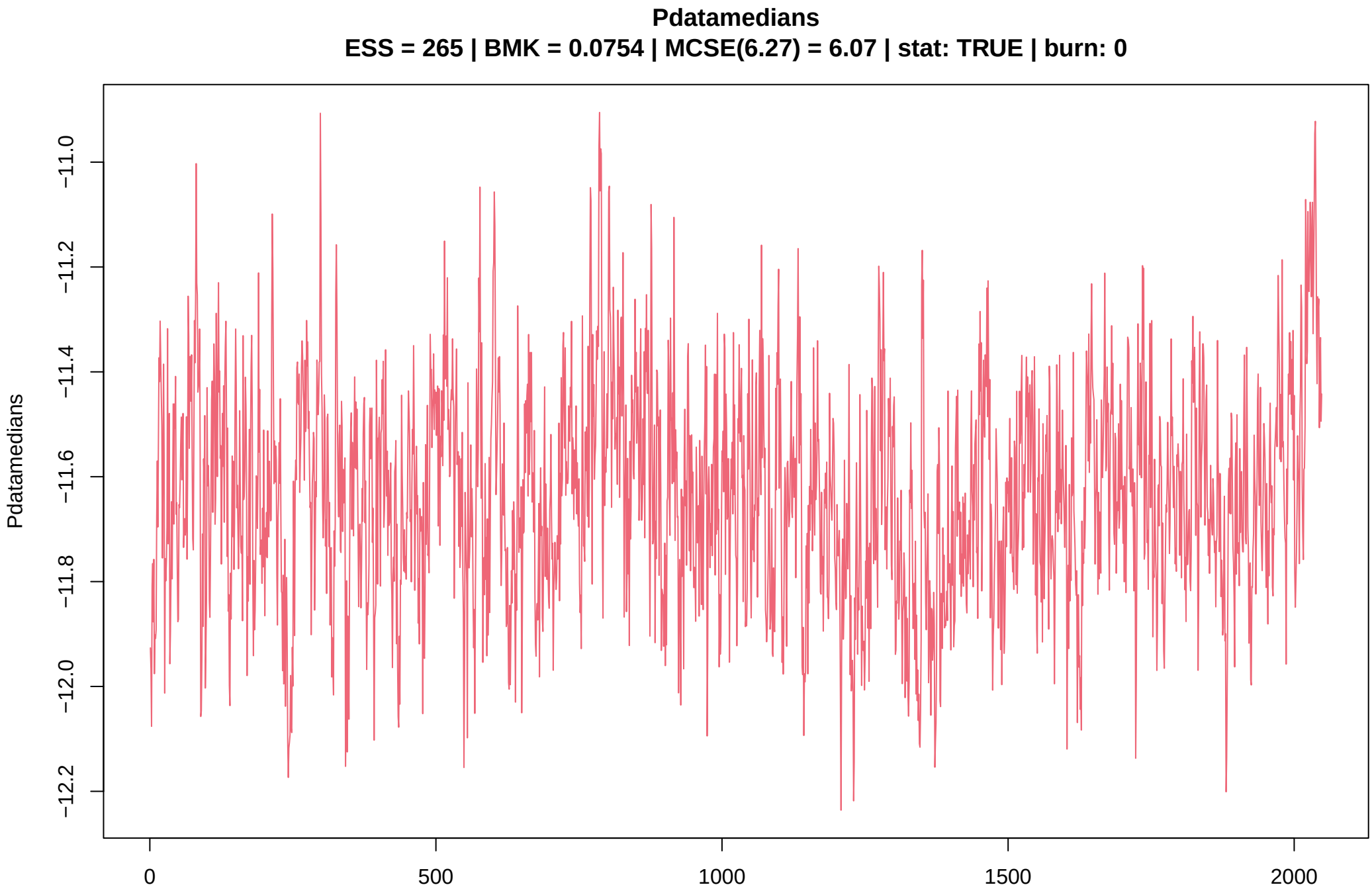

template_HeavyAtomCount
log_RMSD

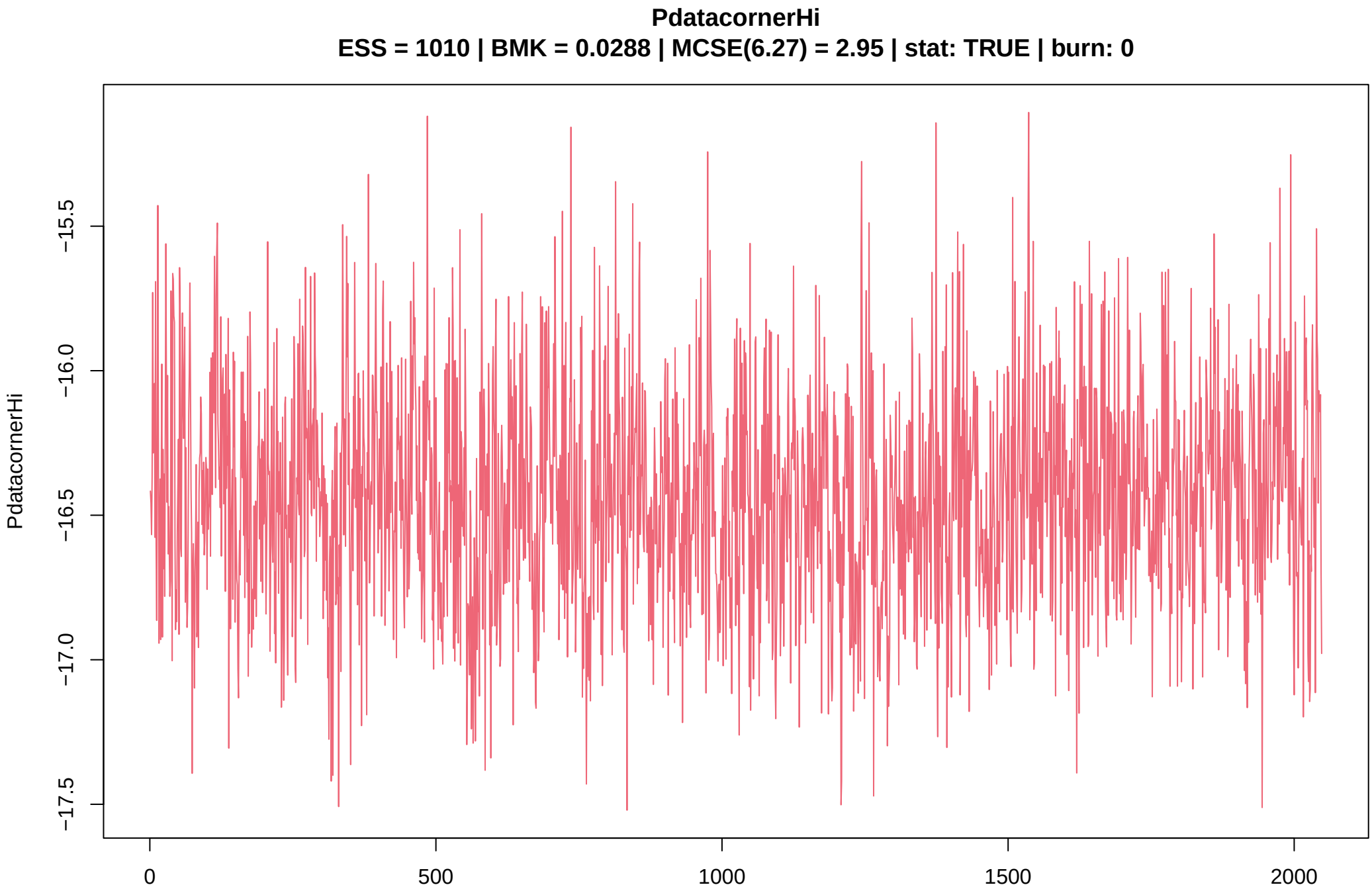

mcs_docked_NumHAcceptors
log_RMSD

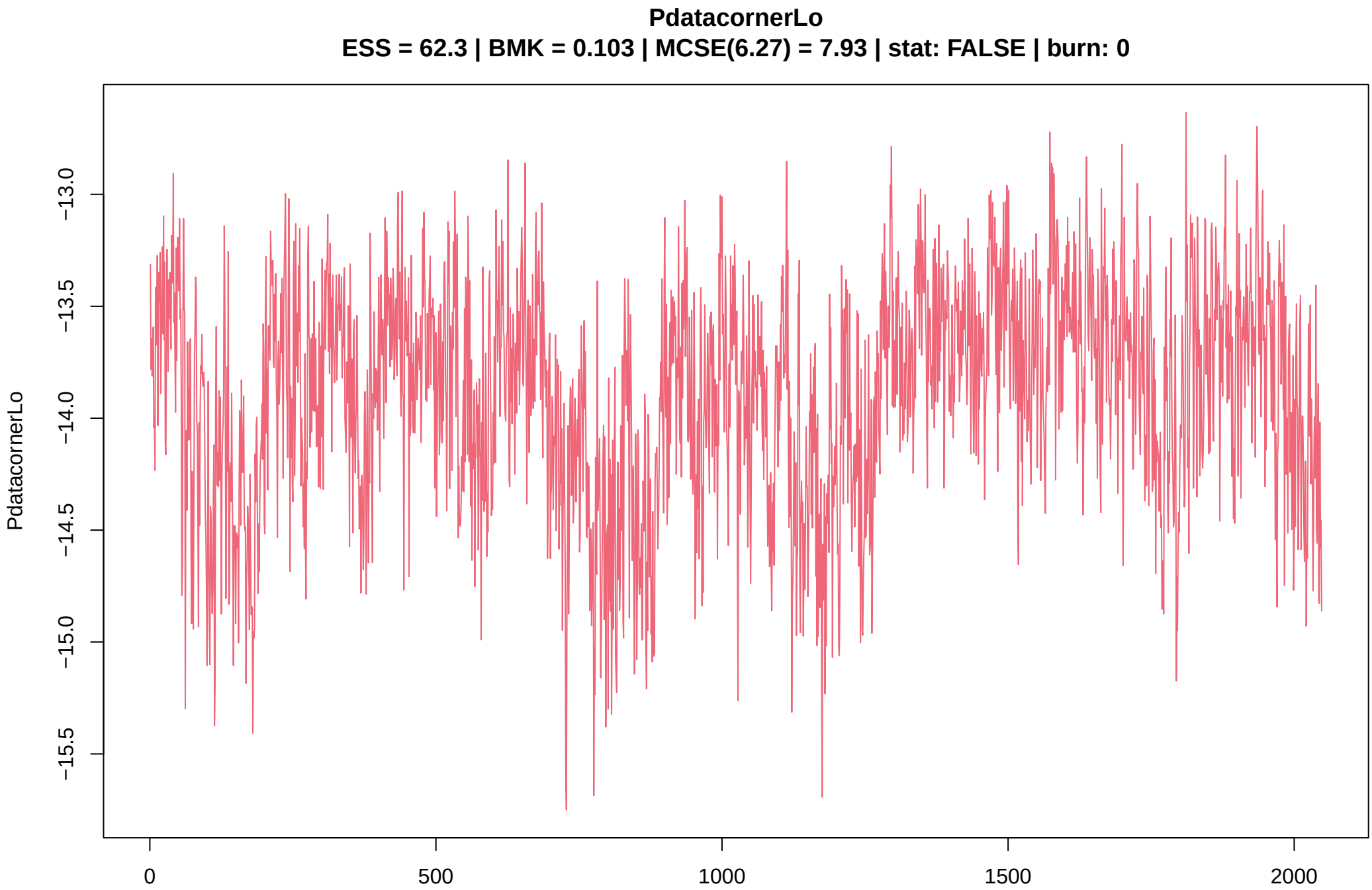

mcs_template_NumHAcceptors
log_RMSD

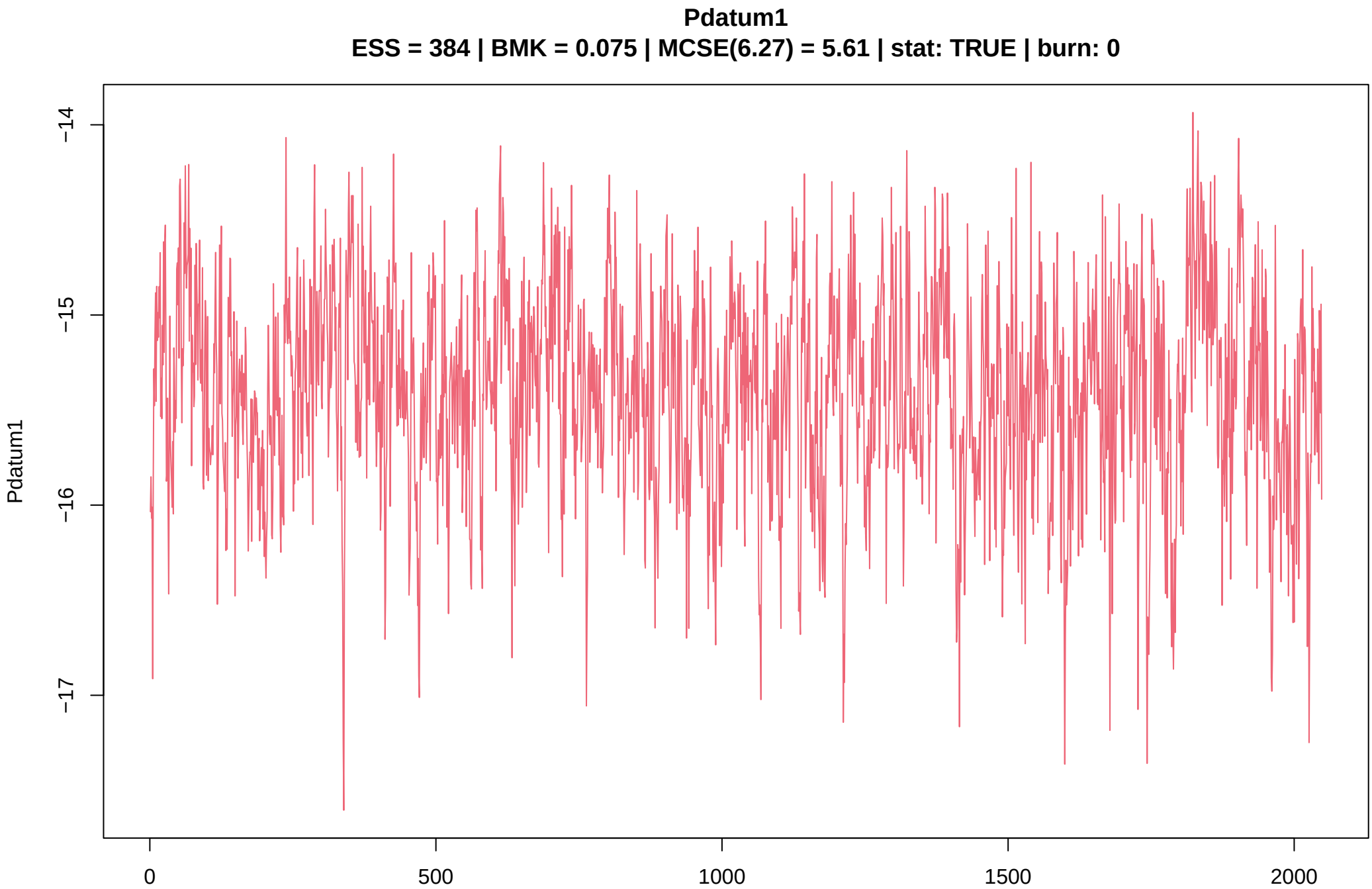

mcs_NumHeteroAtoms
log_RMSD

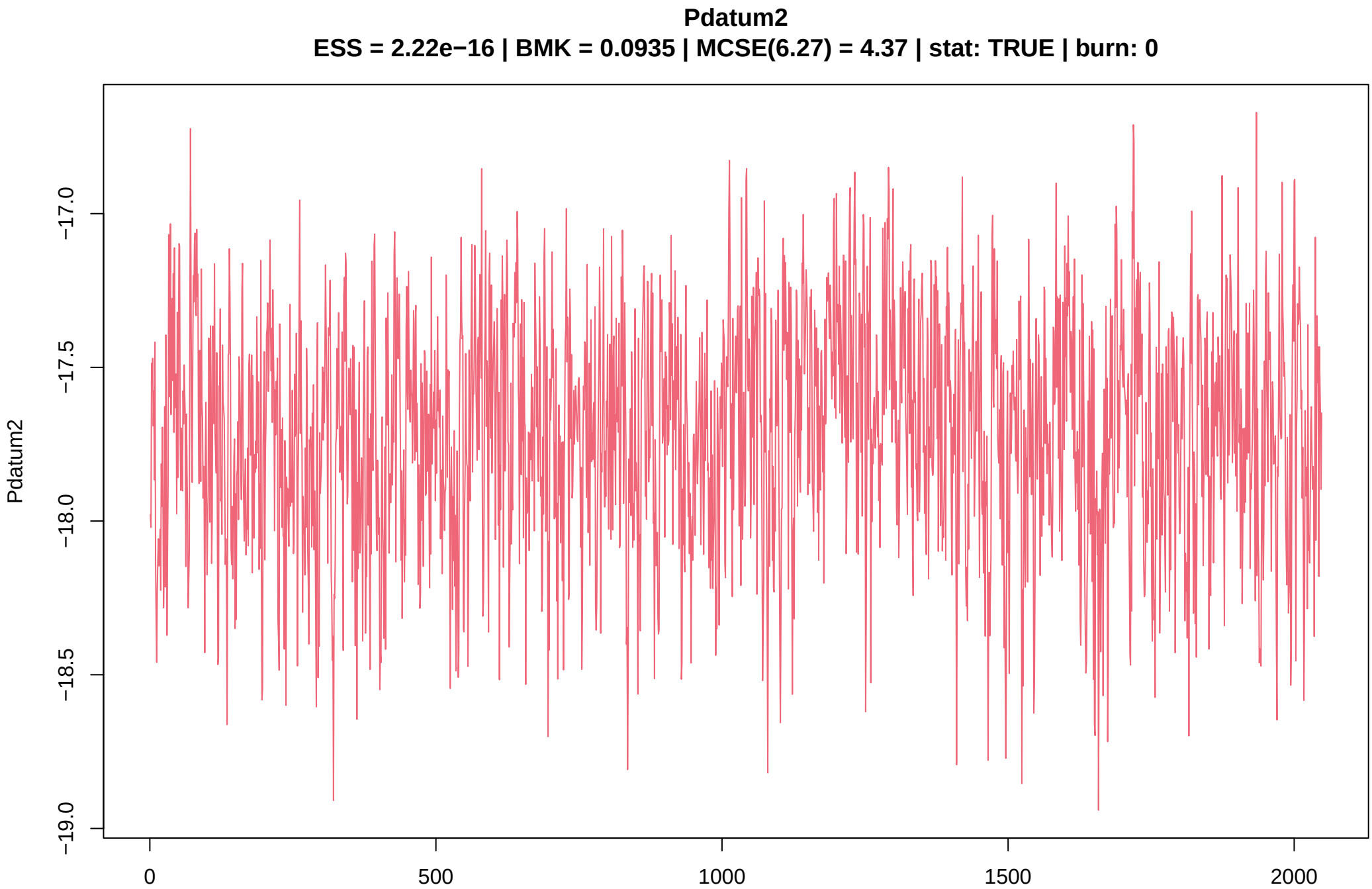

LL
ESS = 78.8 | BMK = 0.0668 | MCSE(6.27) = 8.84 | stat: TRUE | burn: 0
LL
−110150
−110200
−110250
0
500
1000
1500
2000

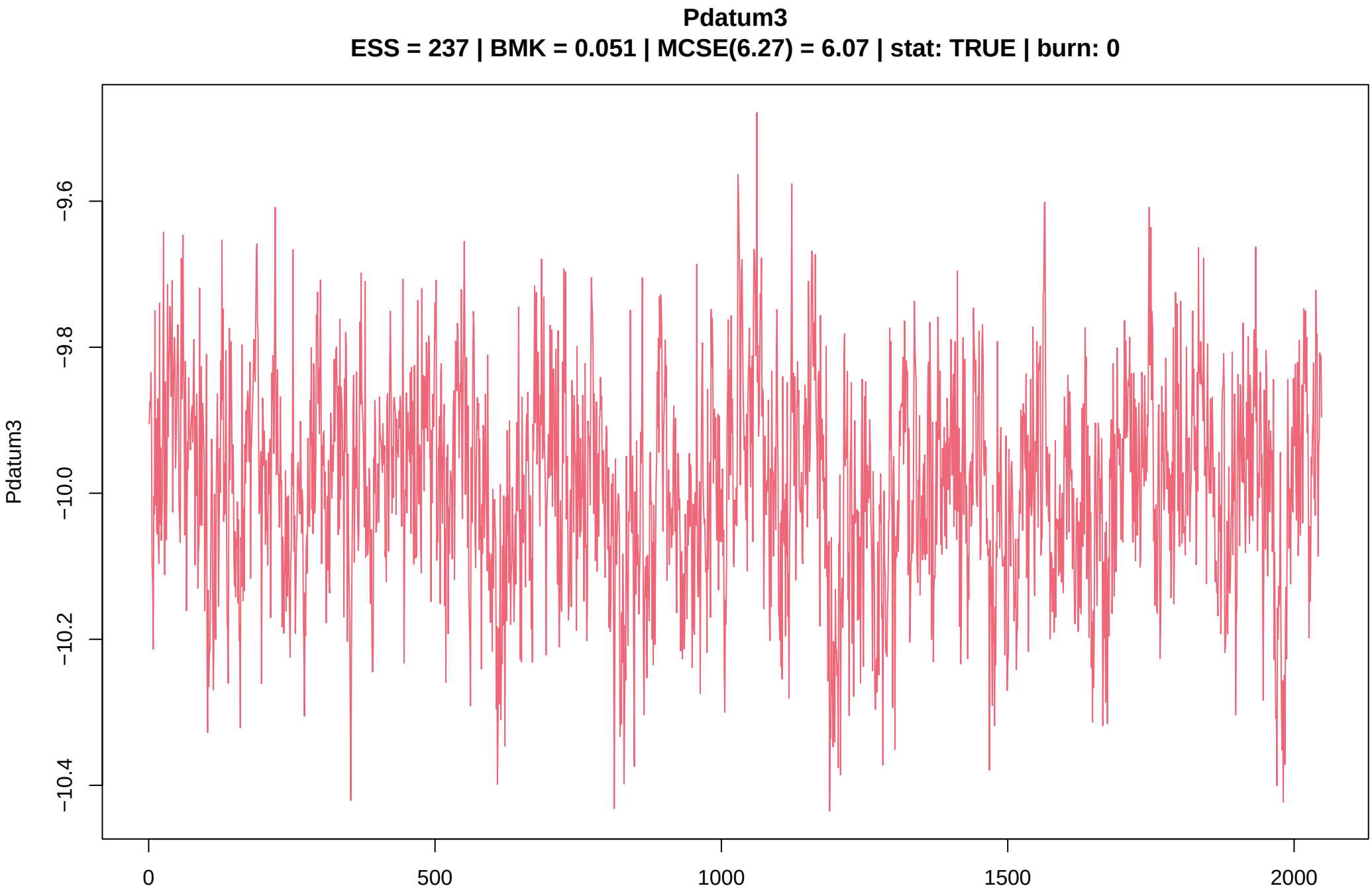

Pdatamedians
ESS = 265 | BMK = 0.0754 | MCSE(6.27) = 6.07 | stat: TRUE | burn: 0
Pdatamedians
−11.0
−11.2
−11.4
−11.6
−11.8
−12.0
−12.2
0
500
1000
1500
2000

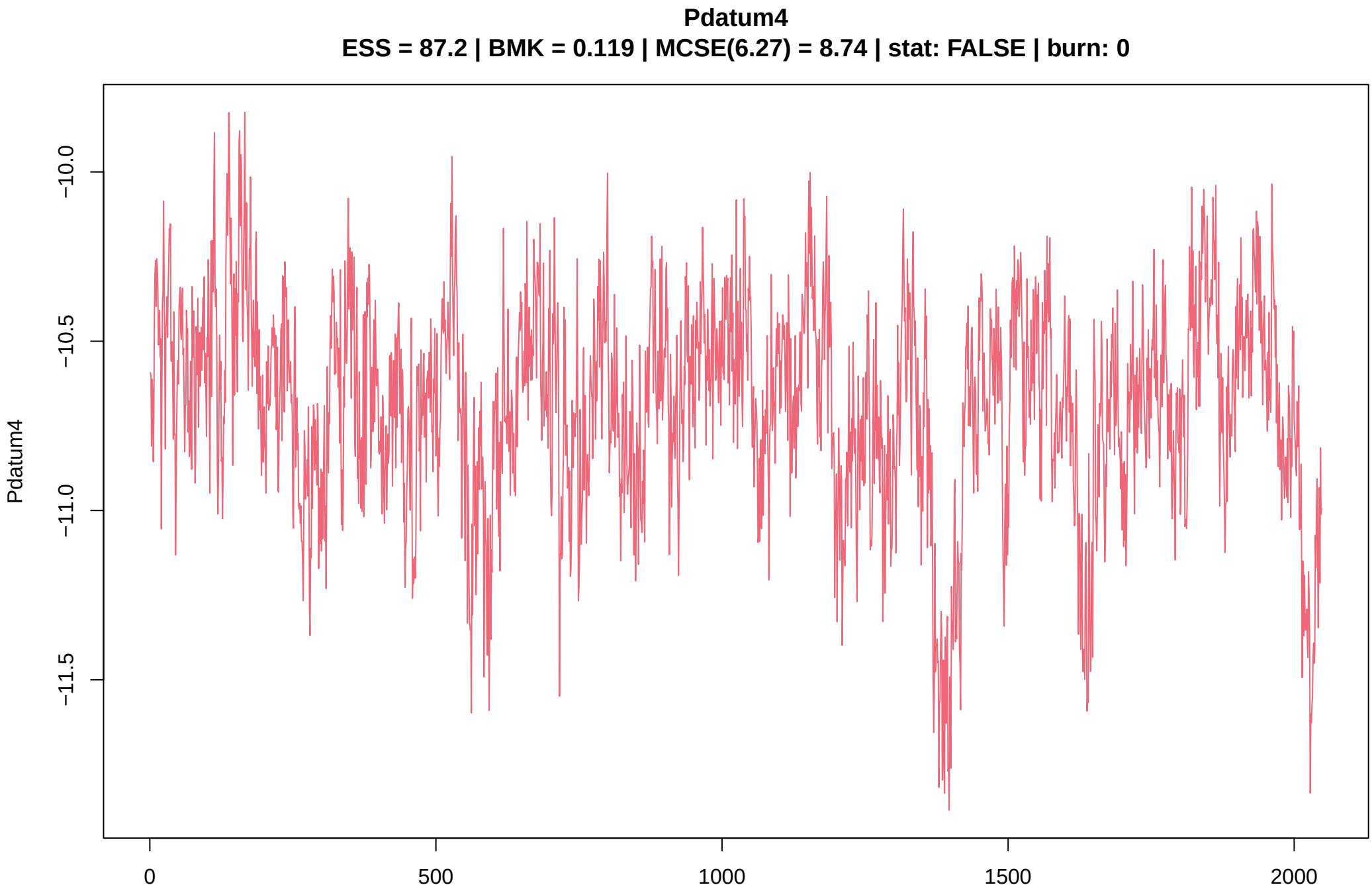

PdatacornerHi
ESS = 1010 | BMK = 0.0288 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0
PdatacornerHi
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

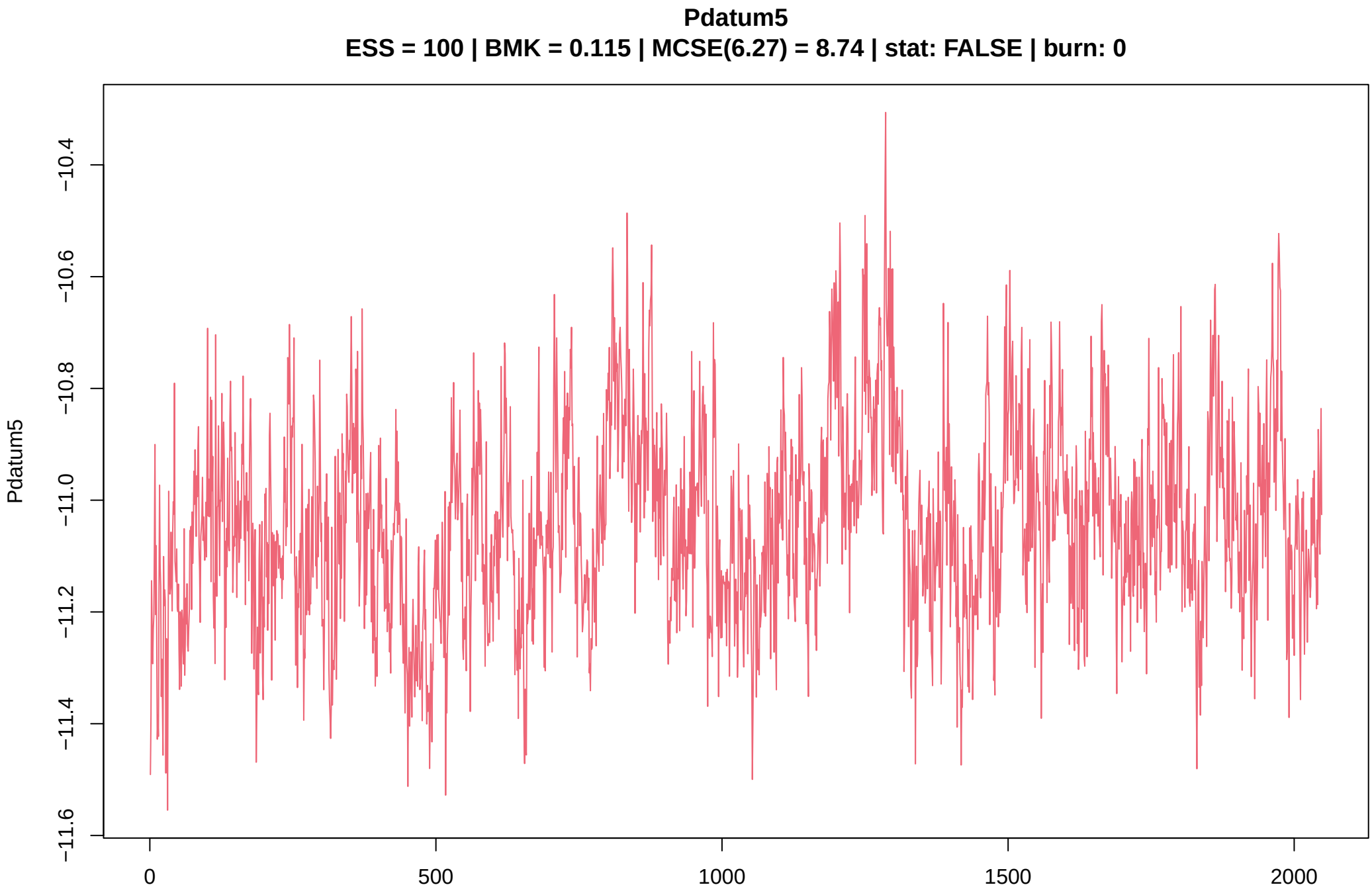

PdatacornerLo
ESS = 62.3 | BMK = 0.103 | MCSE(6.27) = 7.93 | stat: FALSE | burn: 0
PdatacornerLo
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

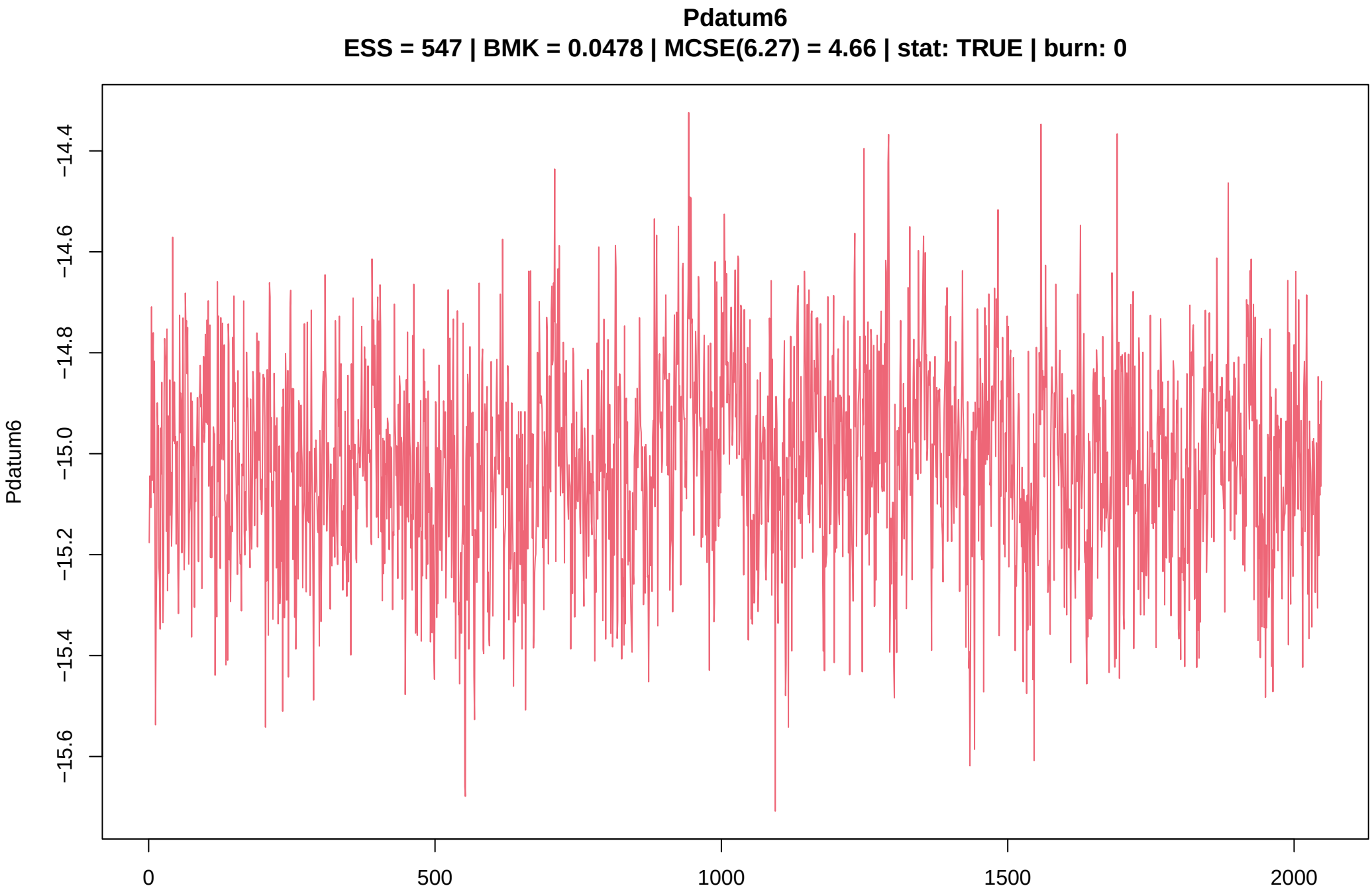

Pdatum1
ESS = 384 | BMK = 0.075 | MCSE(6.27) = 5.61 | stat: TRUE | burn: 0
Pdatum1
−14
−15
−16
−17
0
500
1000
1500
2000

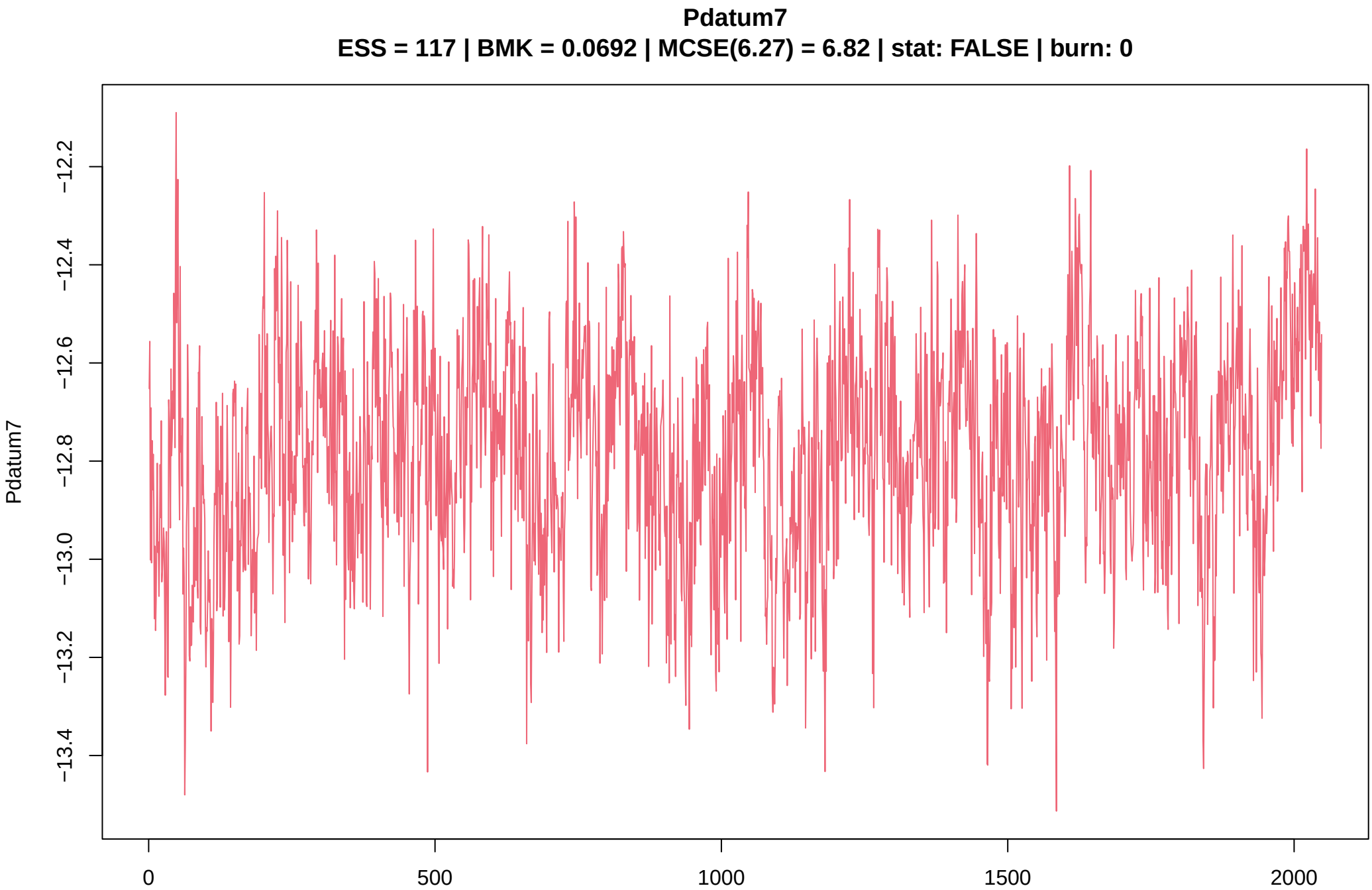

Pdatum2
ESS = 2.22e−16 | BMK = 0.0935 | MCSE(6.27) = 4.37 | stat: TRUE | burn: 0
Pdatum2
−17.0
−17.5
−18.0
−18.5
−19.0
0
500
1000
1500
2000

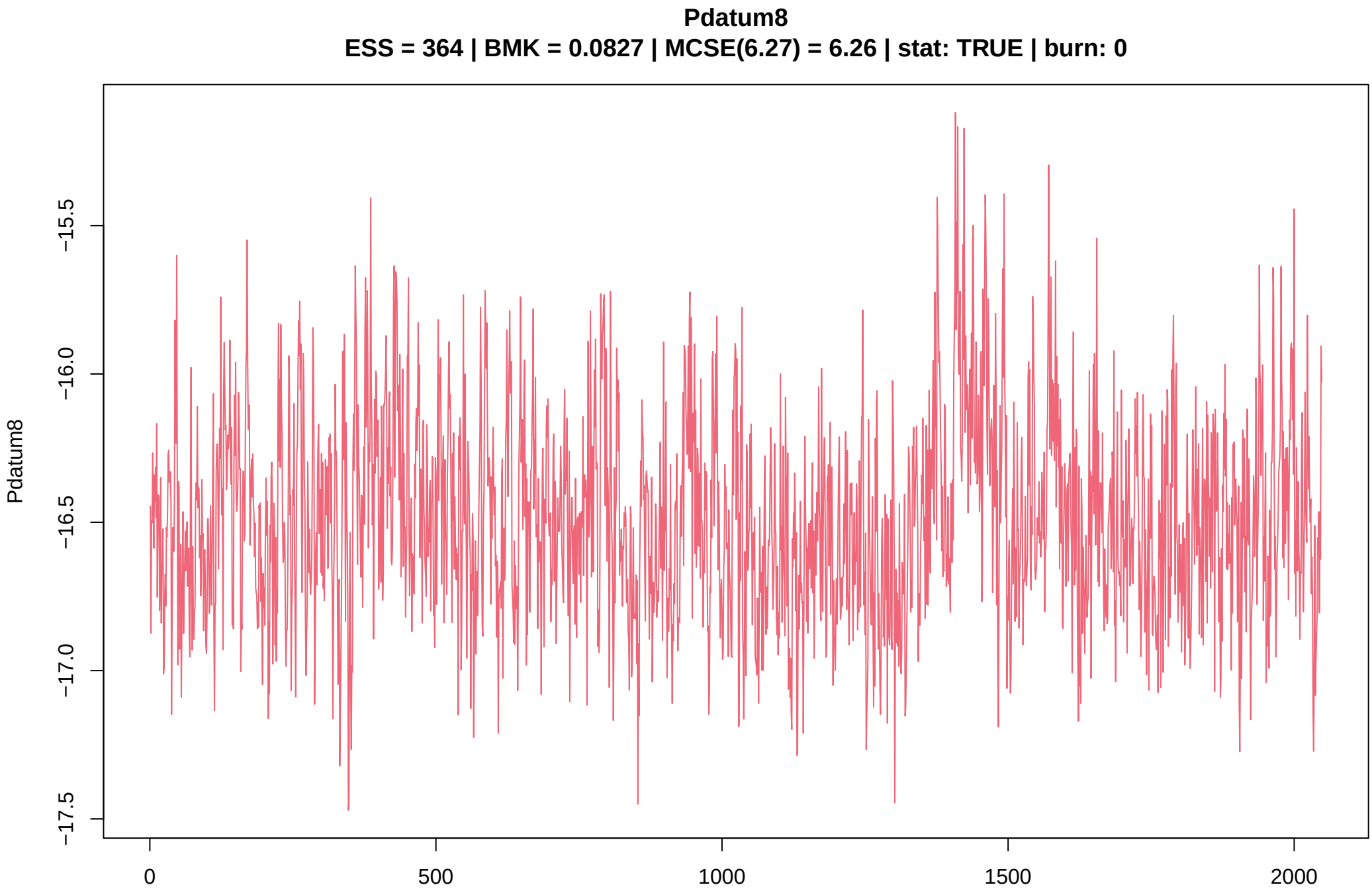

Pdatum3
ESS = 237 | BMK = 0.051 | MCSE(6.27) = 6.07 | stat: TRUE | burn: 0
Pdatum3
−9.6
−9.8
−10.0
−10.2
−10.4
0
500
1000
1500
2000

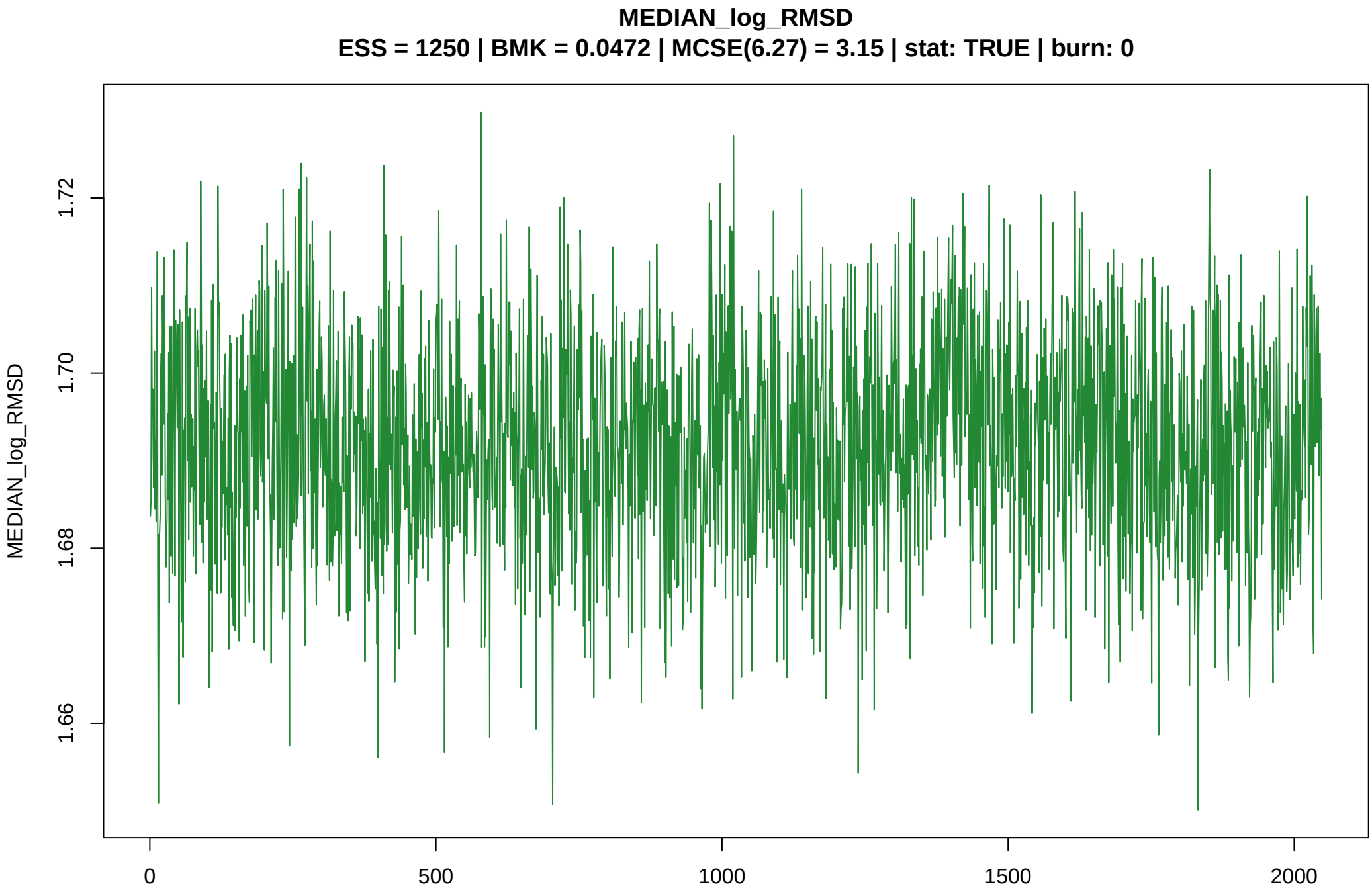

Pdatum4
ESS = 87.2 | BMK = 0.119 | MCSE(6.27) = 8.74 | stat: FALSE | burn: 0
Pdatum4
−10.0
−10.5
−11.0
−11.5
0
500
1000
1500
2000

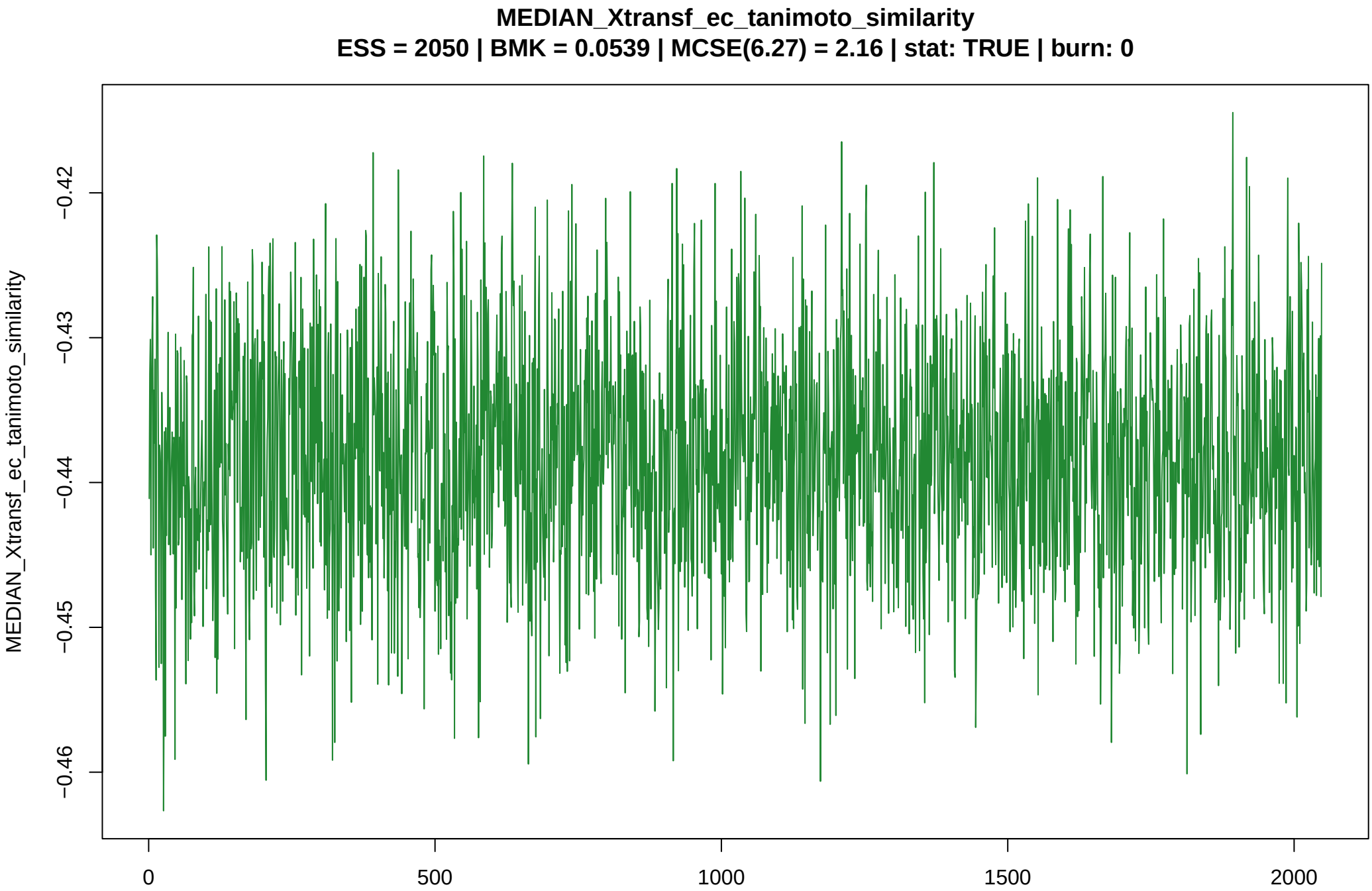

Pdatum5
ESS = 100 | BMK = 0.115 | MCSE(6.27) = 8.74 | stat: FALSE | burn: 0
Pdatum5
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
−11.6
0
500
1000
1500
2000

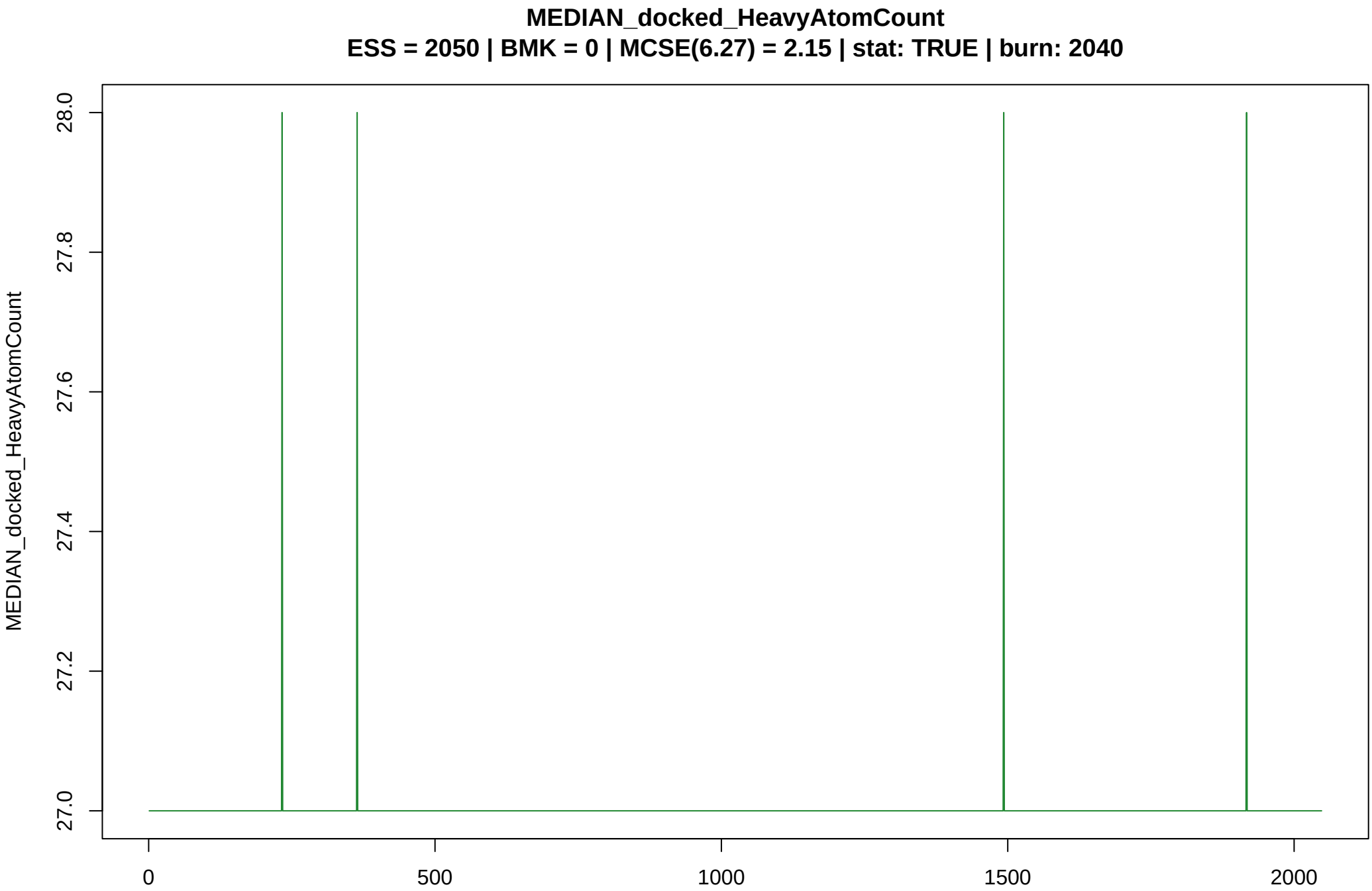

Pdatum6
ESS = 547 | BMK = 0.0478 | MCSE(6.27) = 4.66 | stat: TRUE | burn: 0
Pdatum6
−14.4
−14.6
−14.8
−15.0
−15.2
−15.4
−15.6
0
500
1000
1500
2000

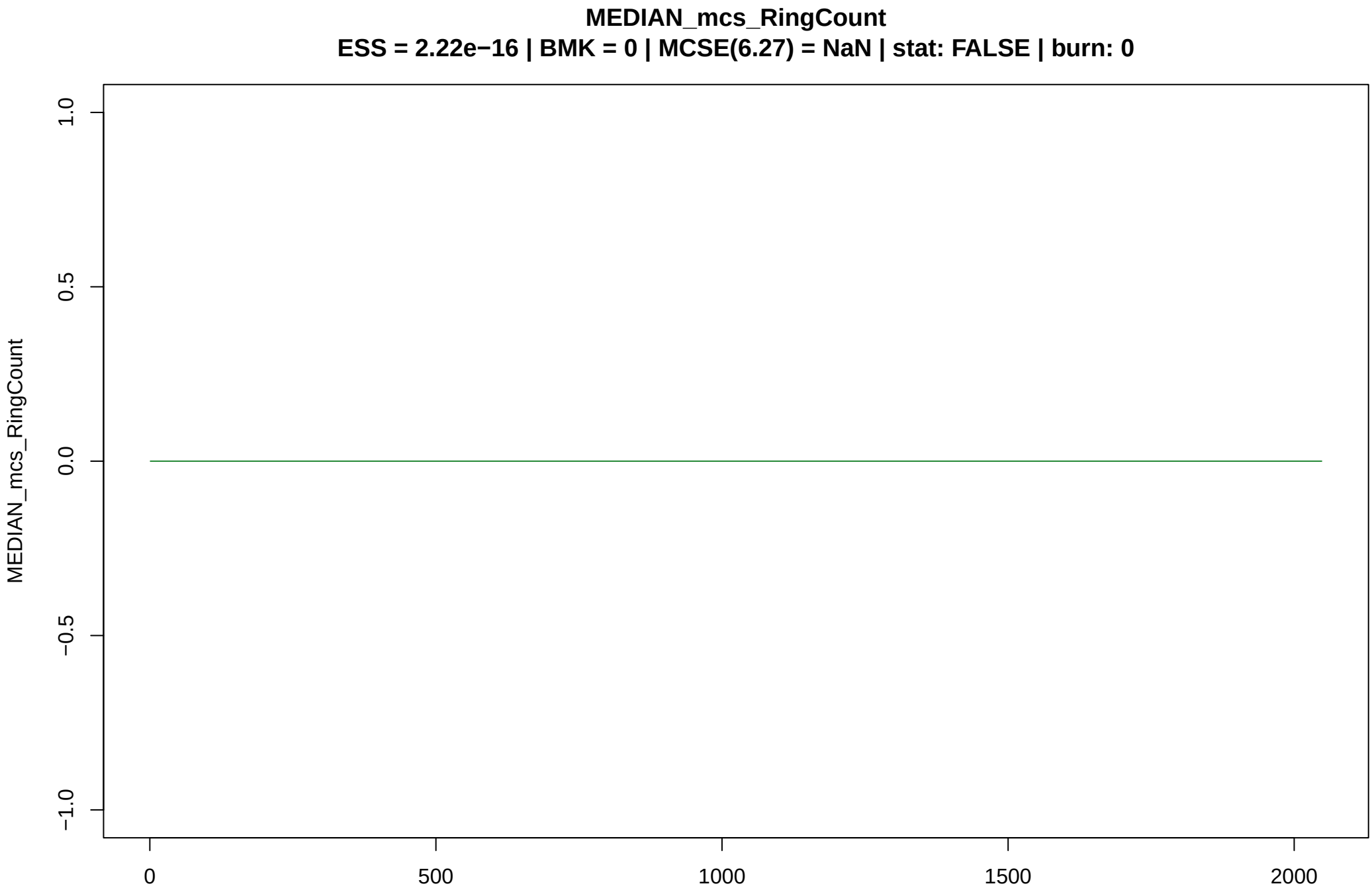

Pdatum7
ESS = 117 | BMK = 0.0692 | MCSE(6.27) = 6.82 | stat: FALSE | burn: 0
Pdatum7
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
−13.4
0
500
1000
1500
2000

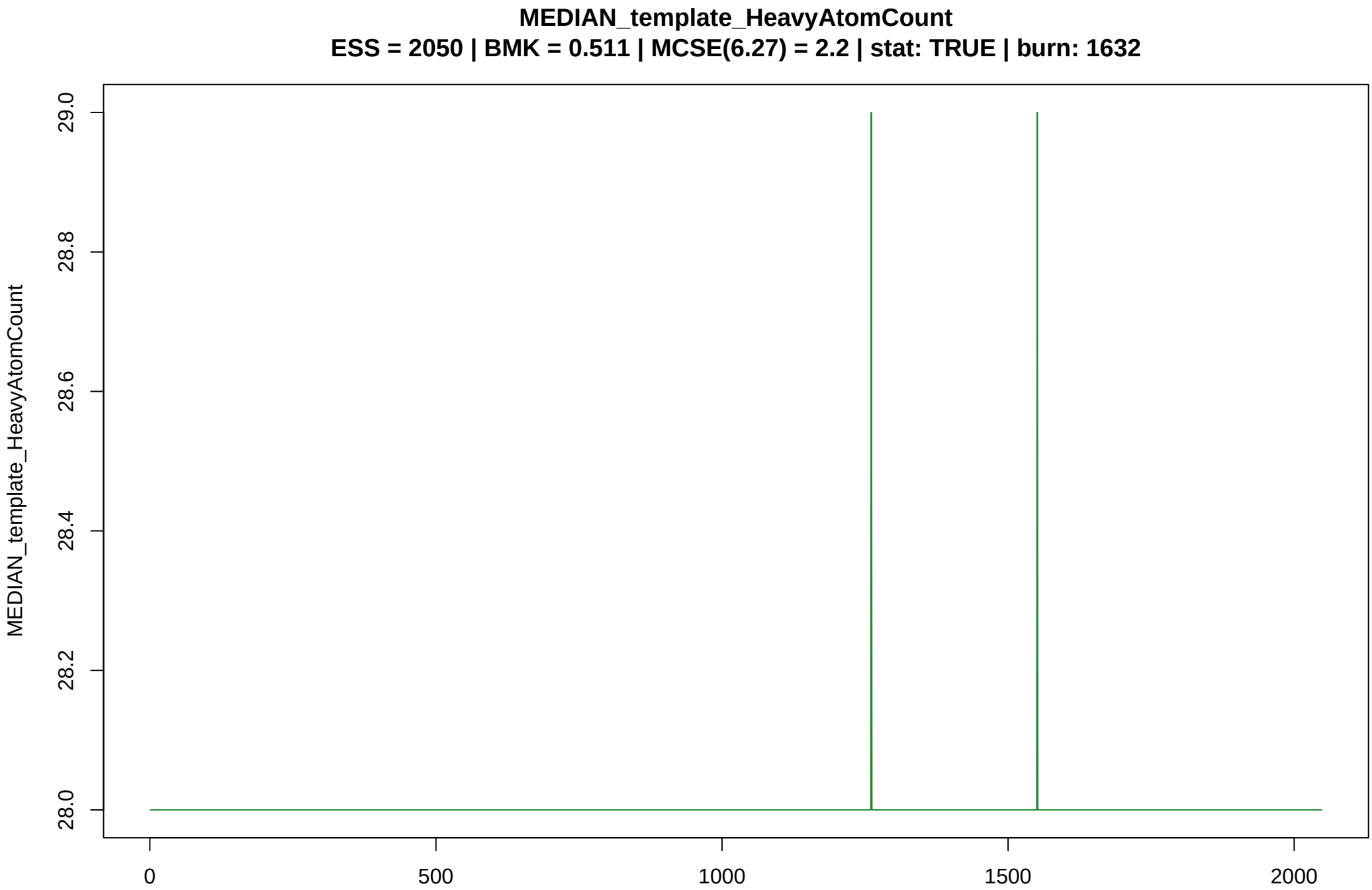

Pdatum8
ESS = 364 | BMK = 0.0827 | MCSE(6.27) = 6.26 | stat: TRUE | burn: 0
Pdatum8
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

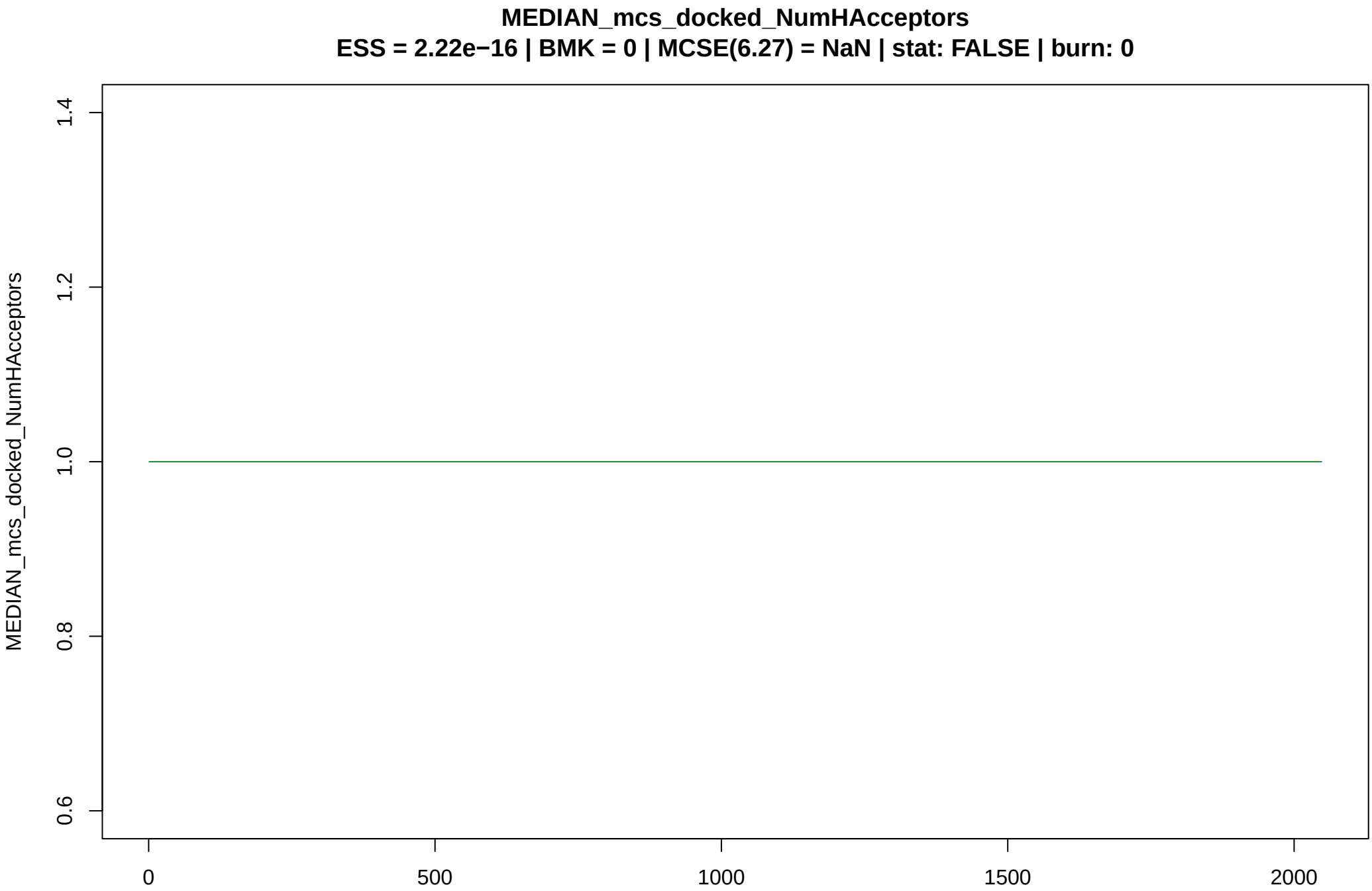

MEDIAN_log_RMSD
ESS = 1250 | BMK = 0.0472 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

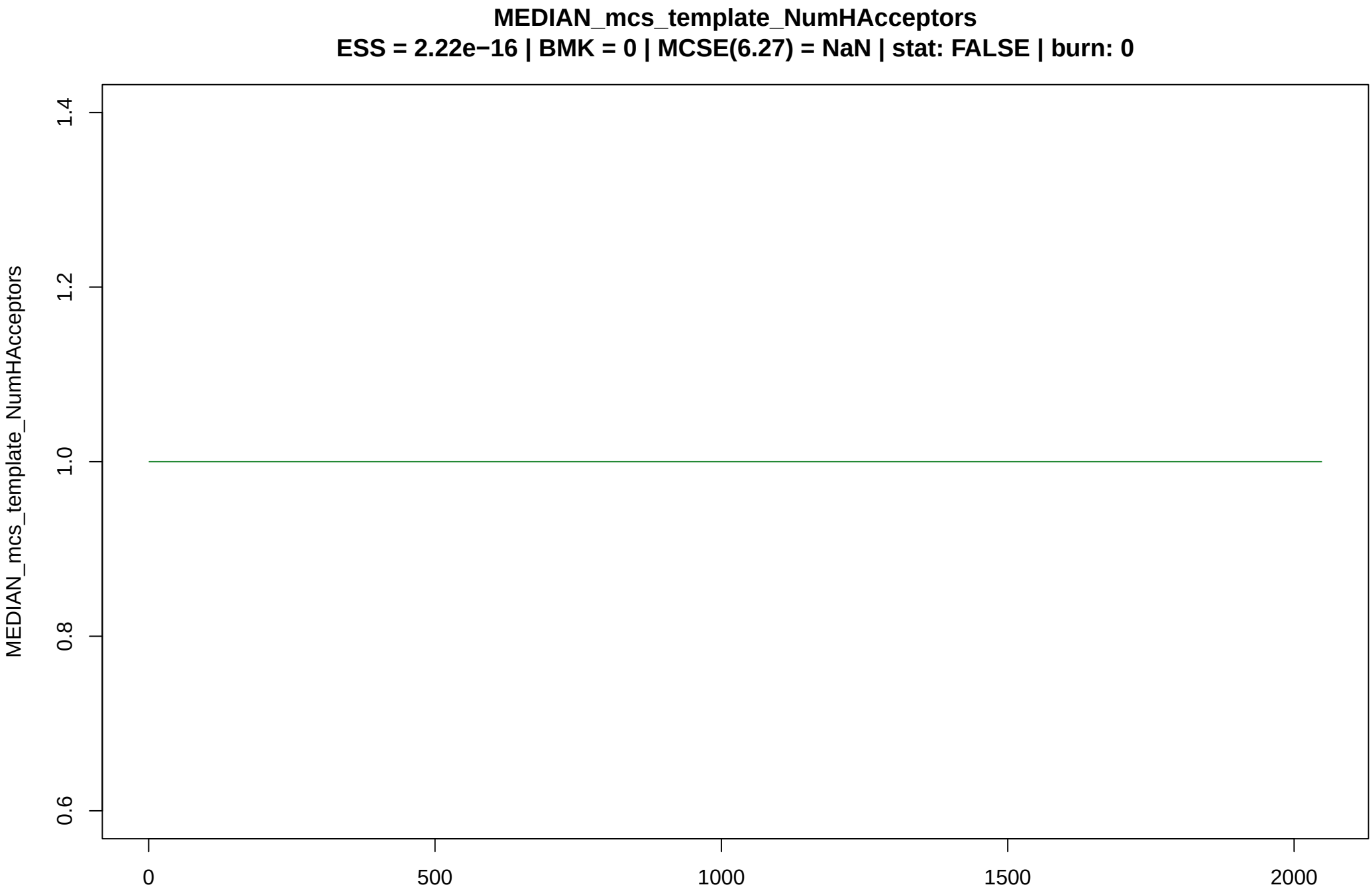

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0539 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

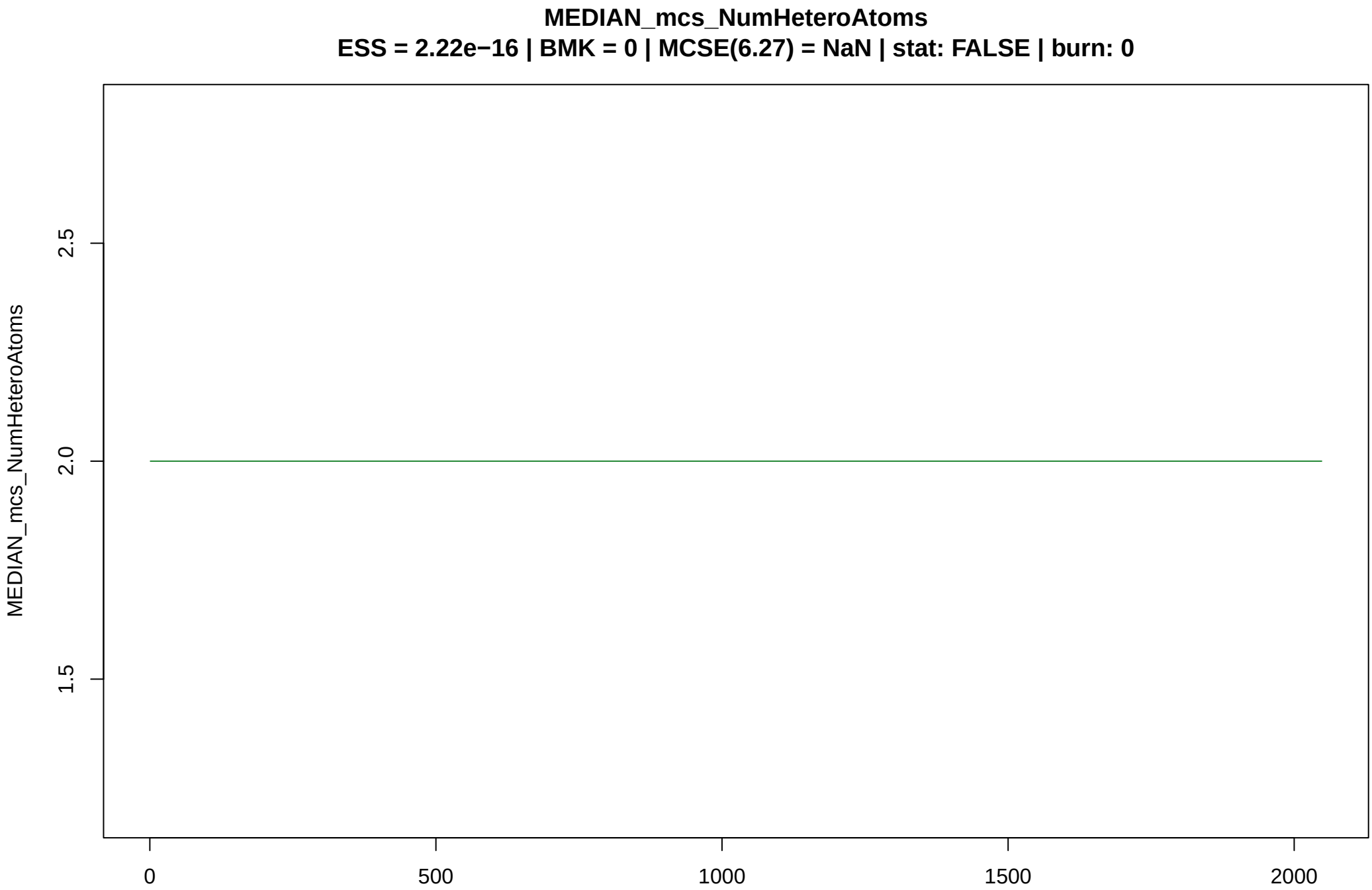

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 2040
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

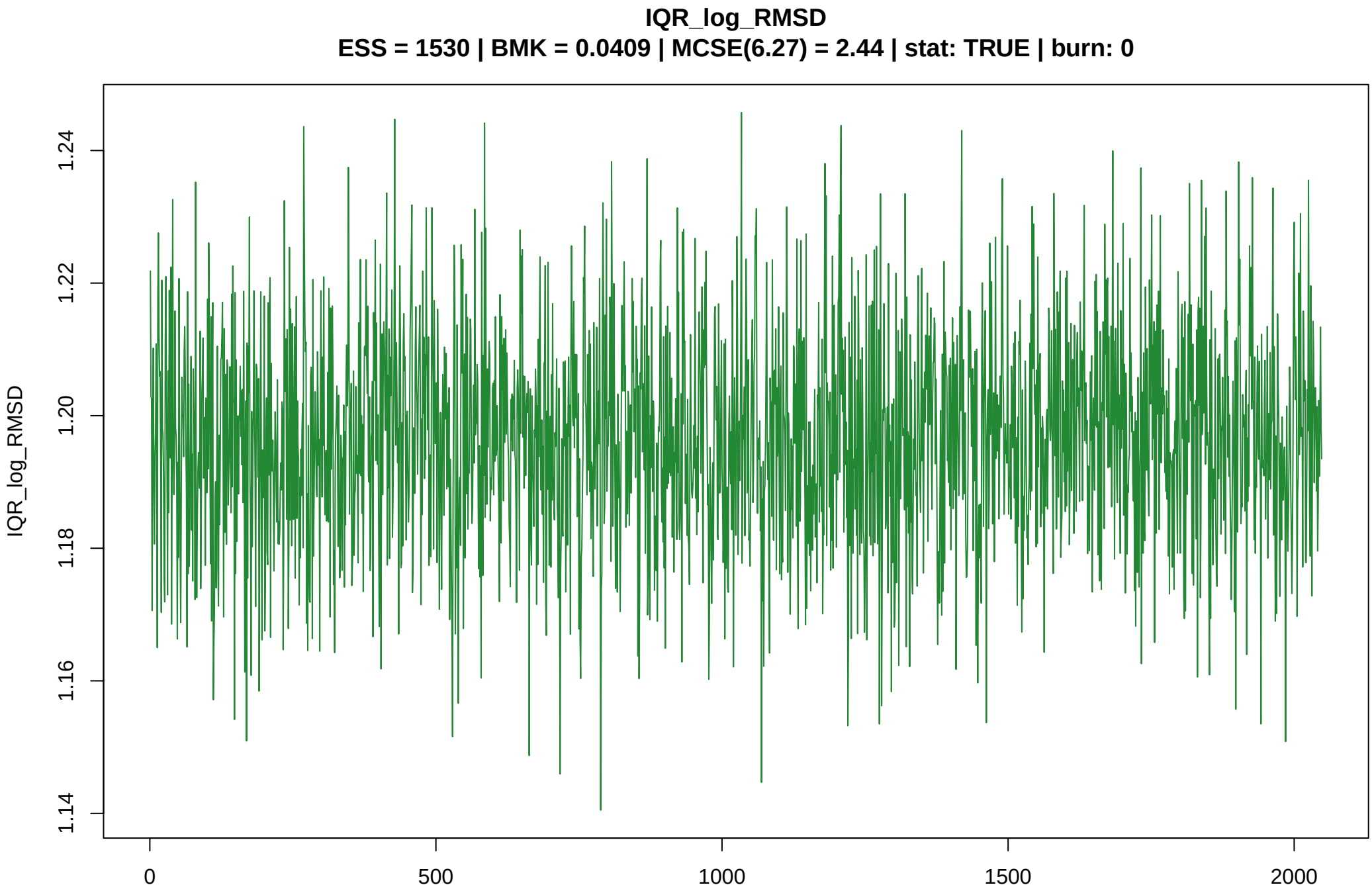

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

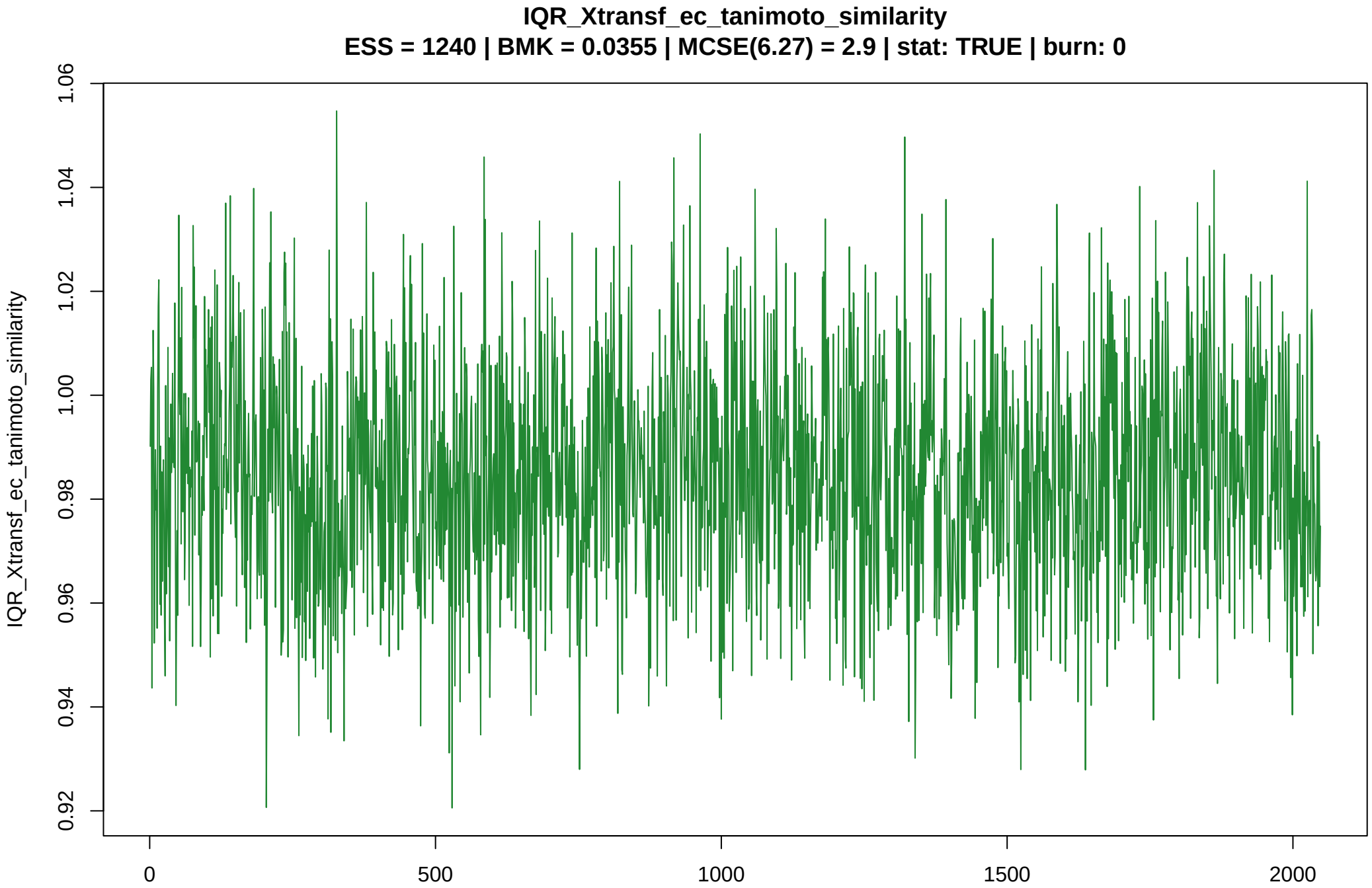

MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.511 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

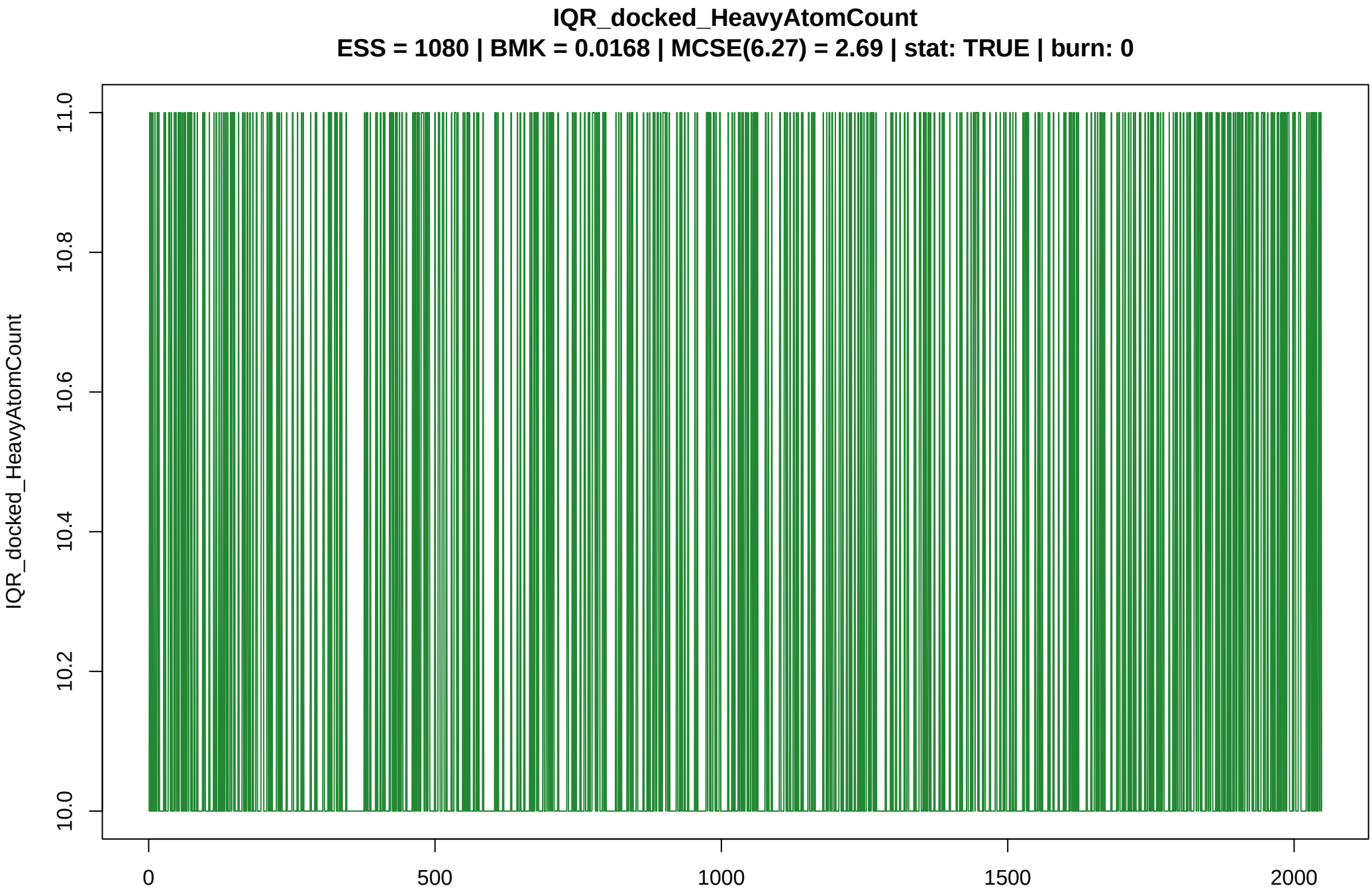

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

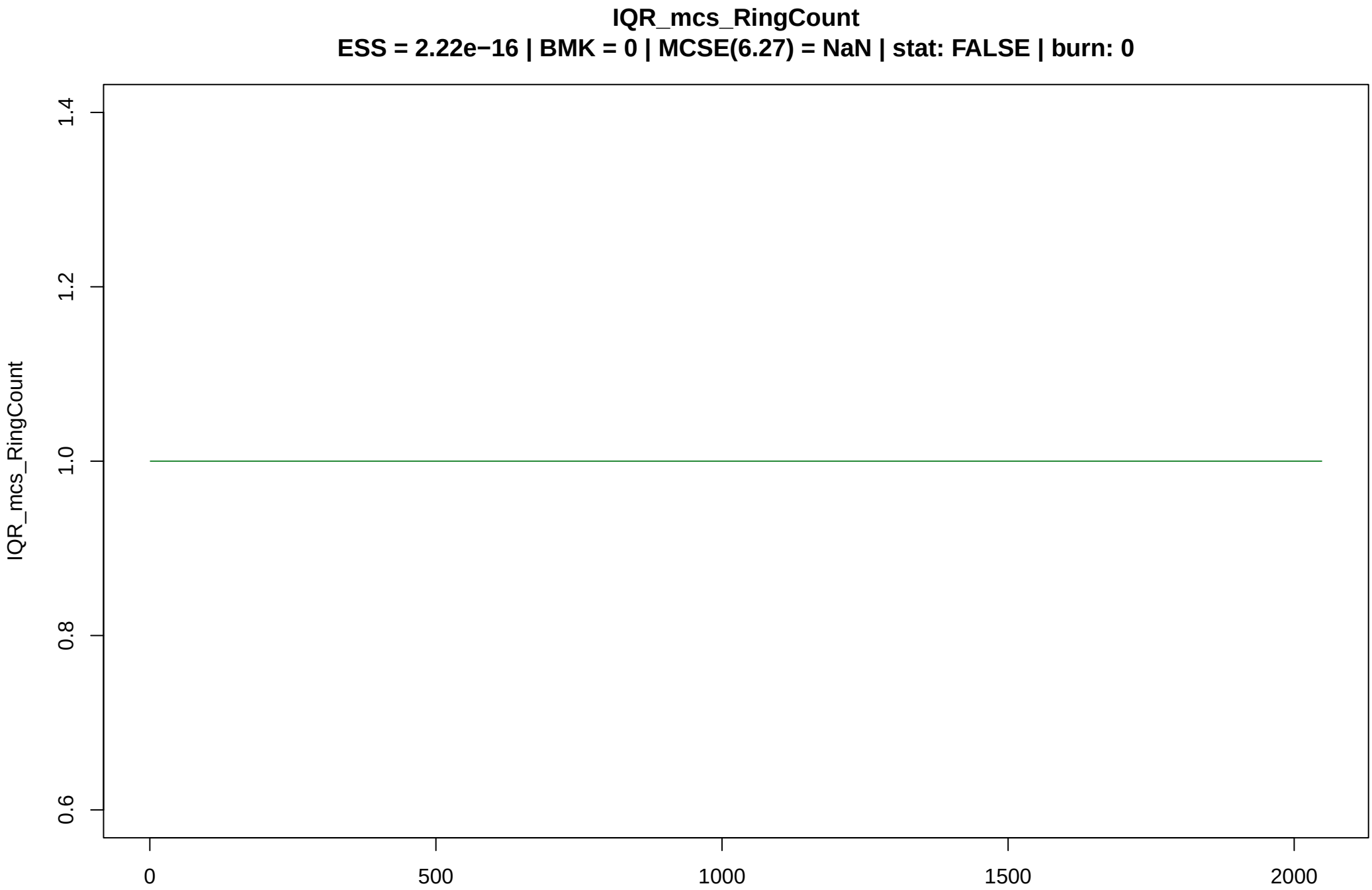

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

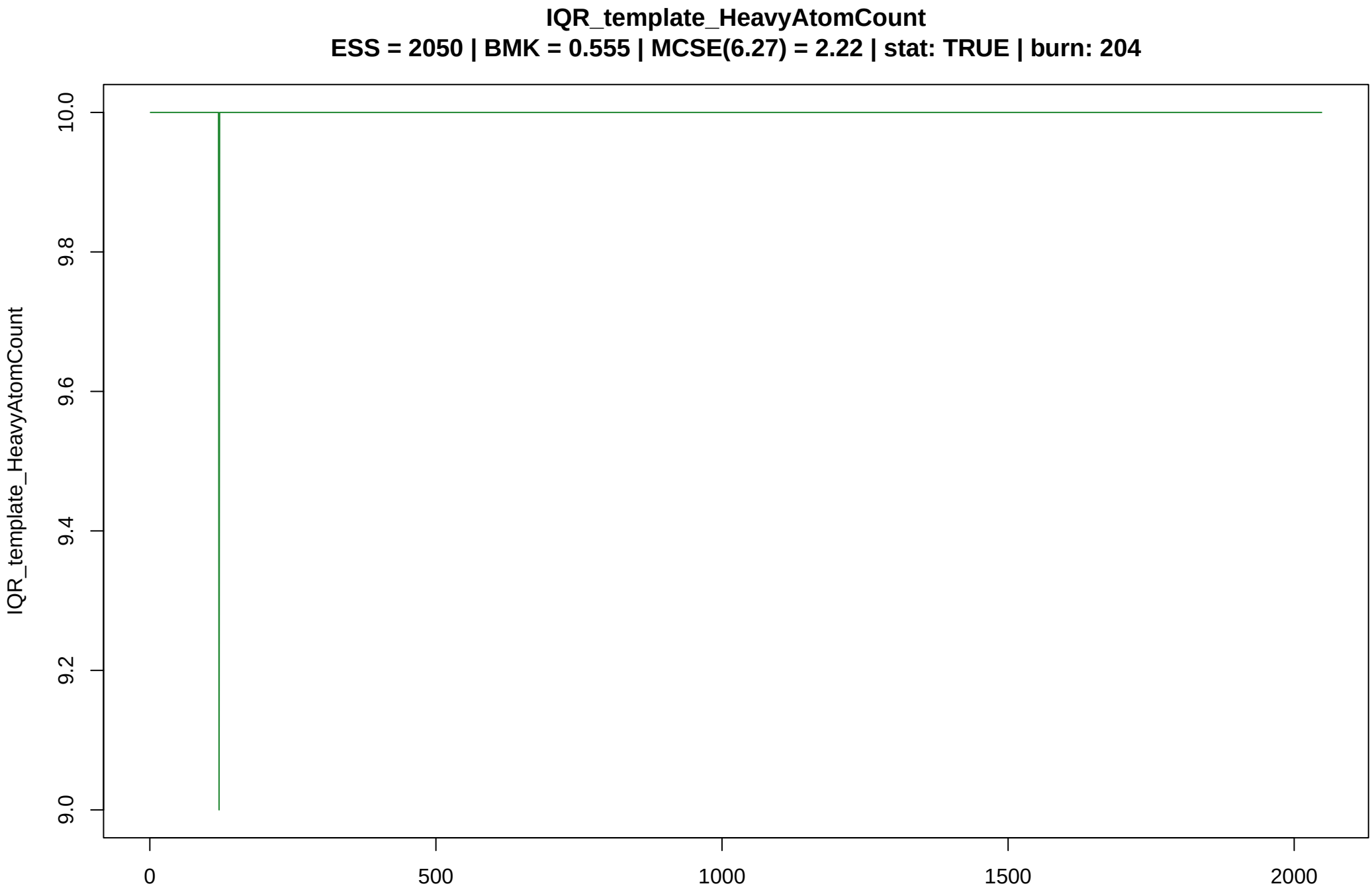

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

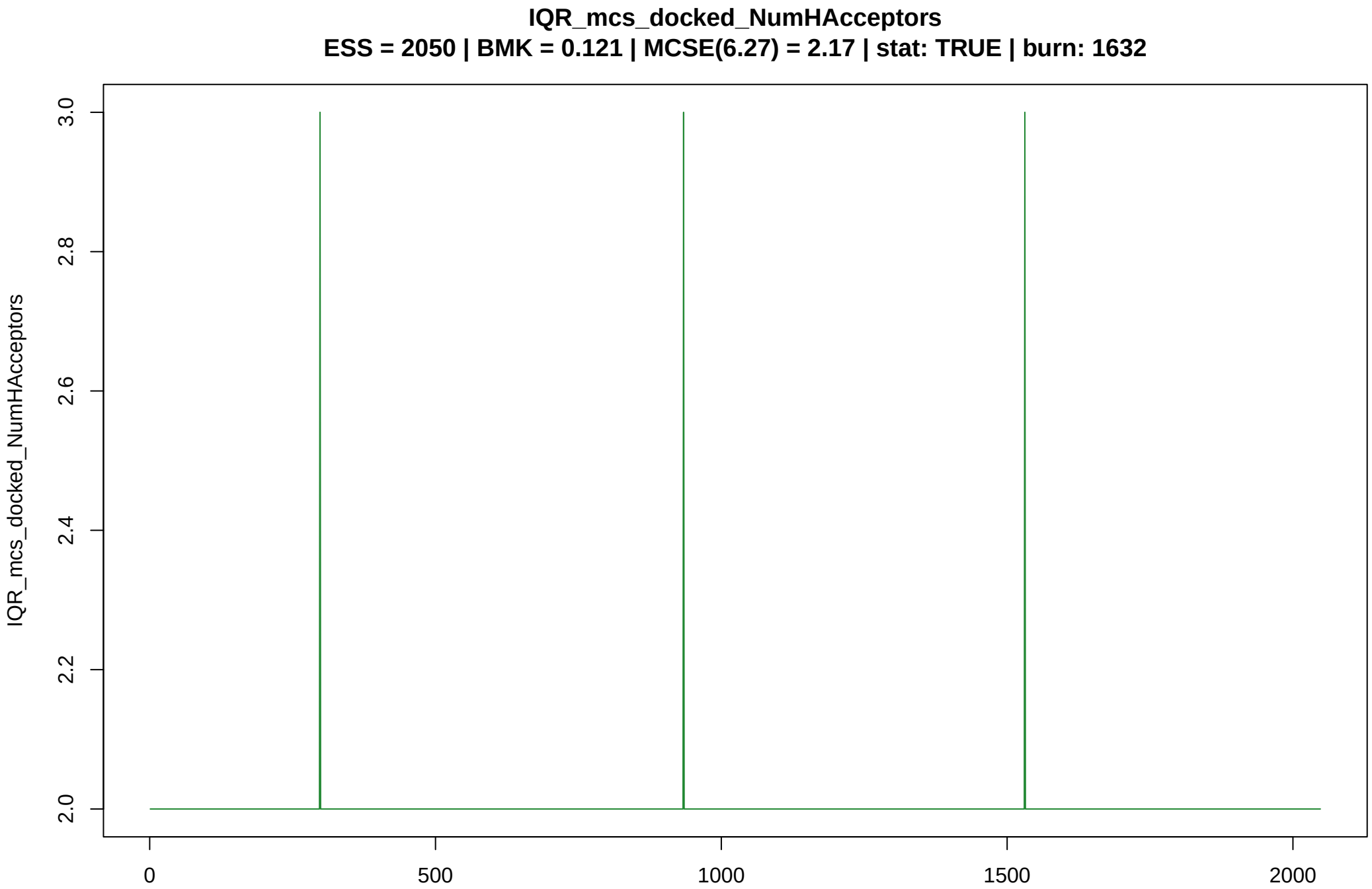

IQR_log_RMSD
ESS = 1530 | BMK = 0.0409 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0
IQR_log_RMSD
1.14
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

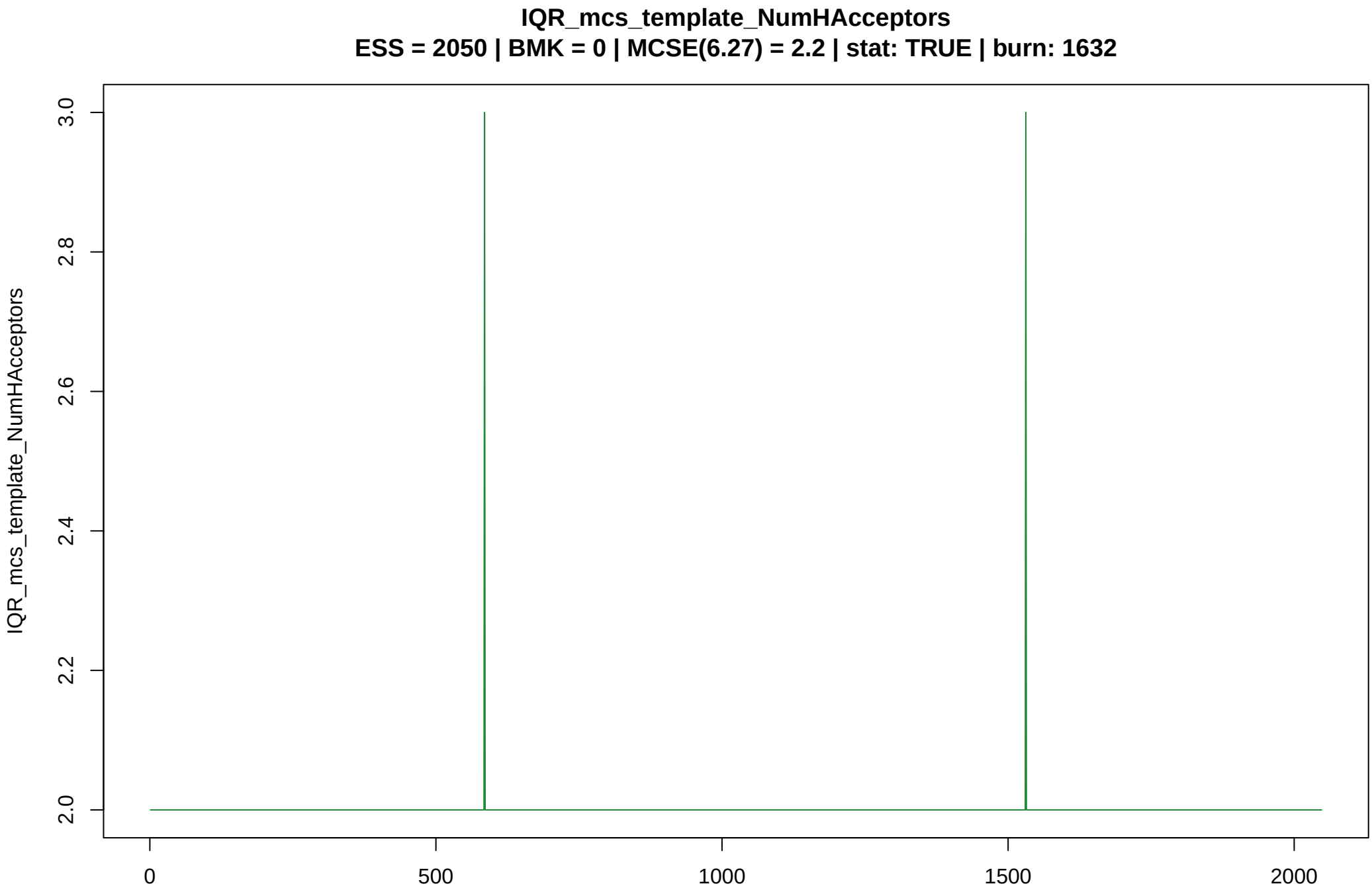

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1240 | BMK = 0.0355 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.92
0.94
0.96
0.98
1.00
1.02
1.04
1.06
0
500
1000
1500
2000

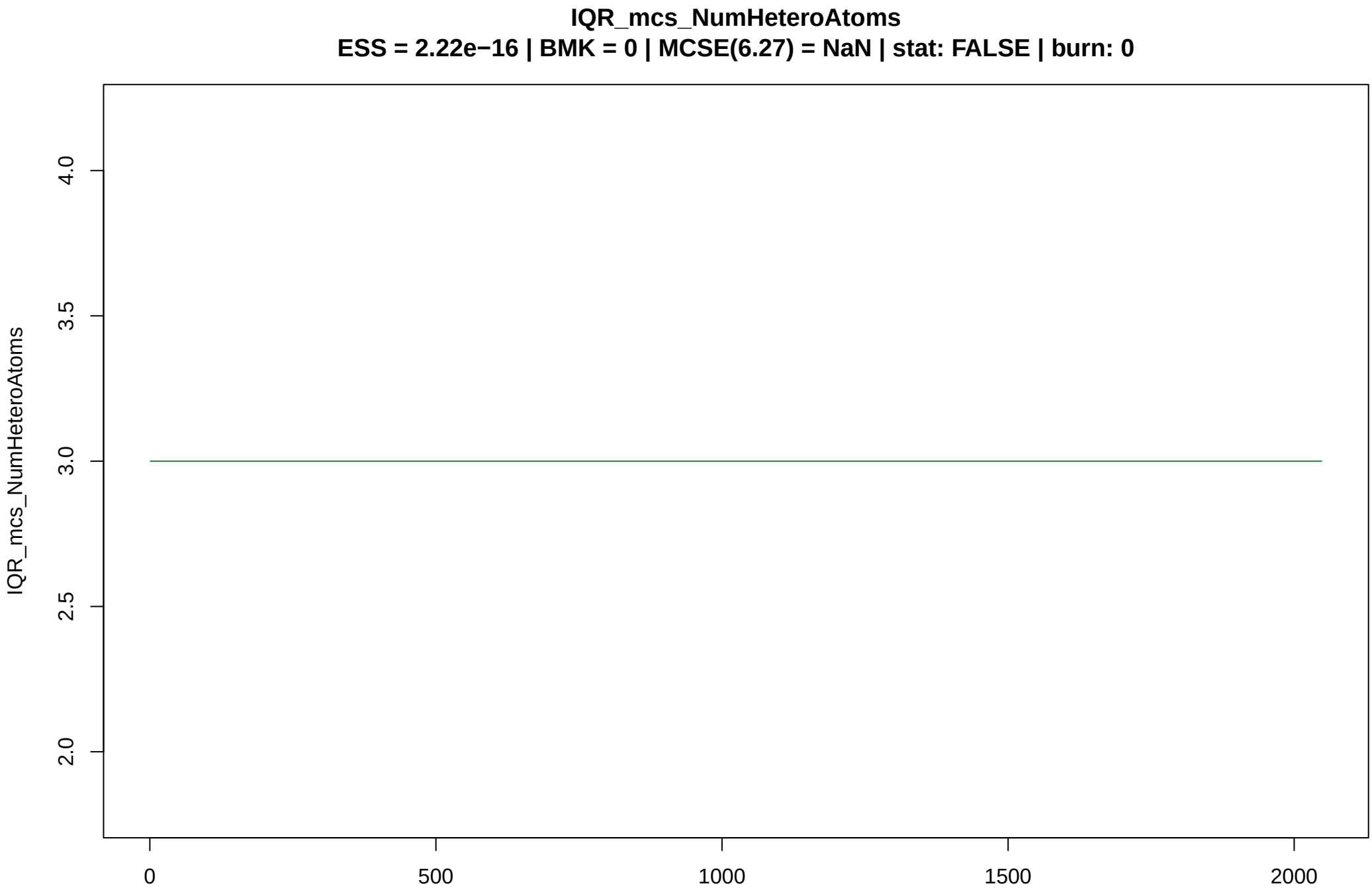

IQR_docked_HeavyAtomCount
ESS = 1080 | BMK = 0.0168 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
10.0
10.2
10.4
10.6
10.8
11.0
0
500
1000
1500
2000

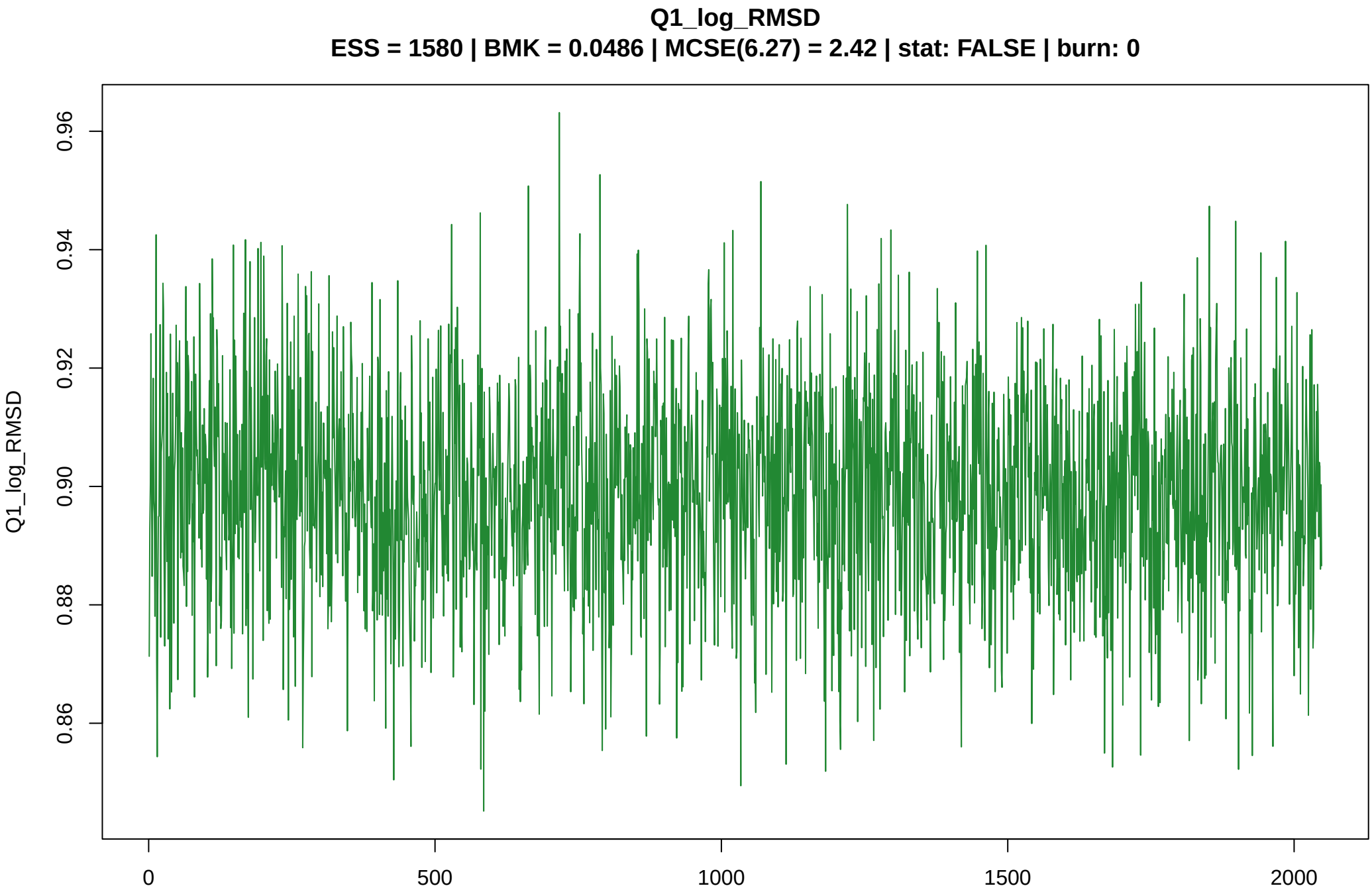

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

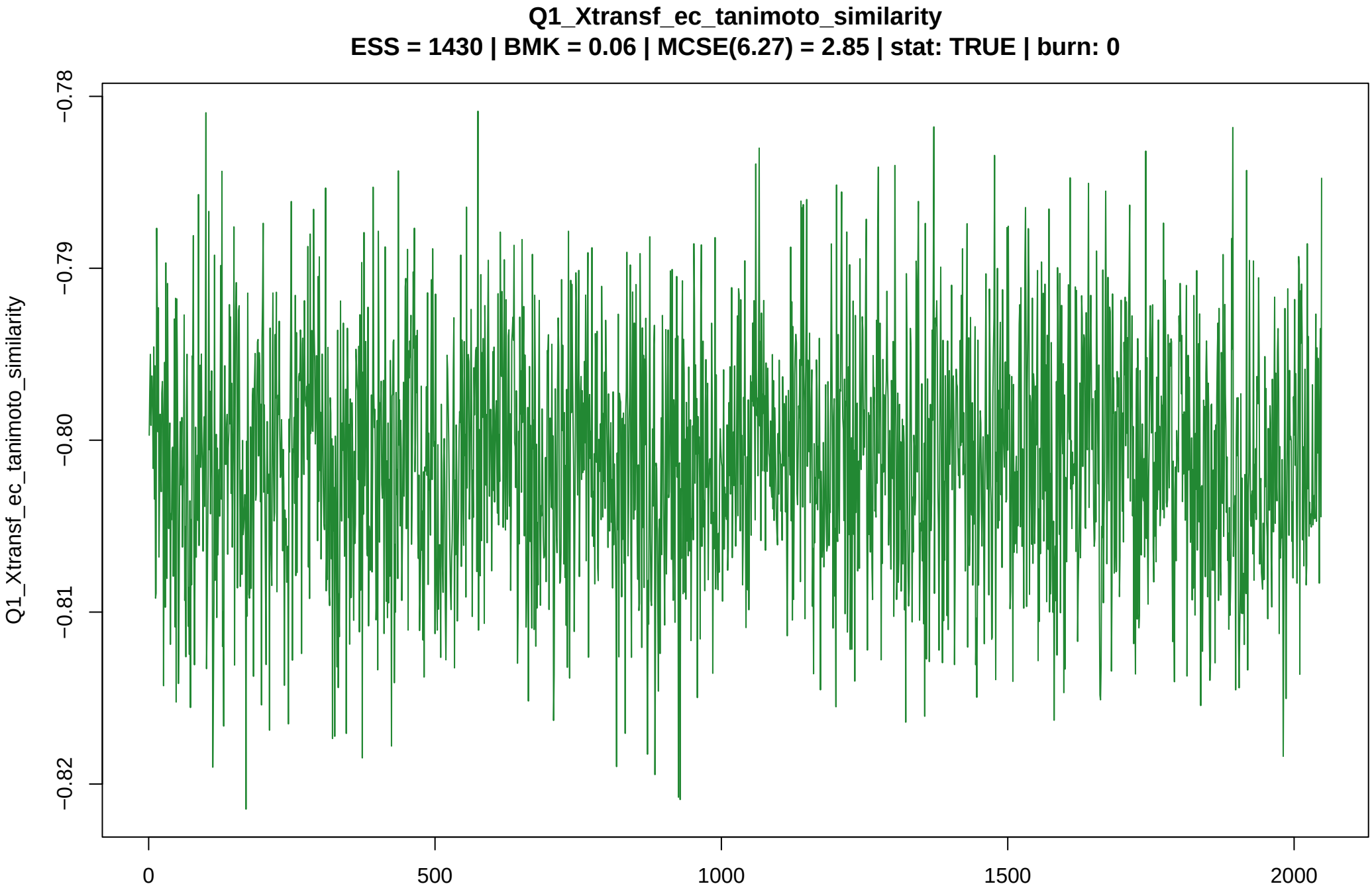

IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.555 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204
IQR_template_HeavyAtomCount
10.0
9.8
9.6
9.4
9.2
9.0
0
500
1000
1500
2000

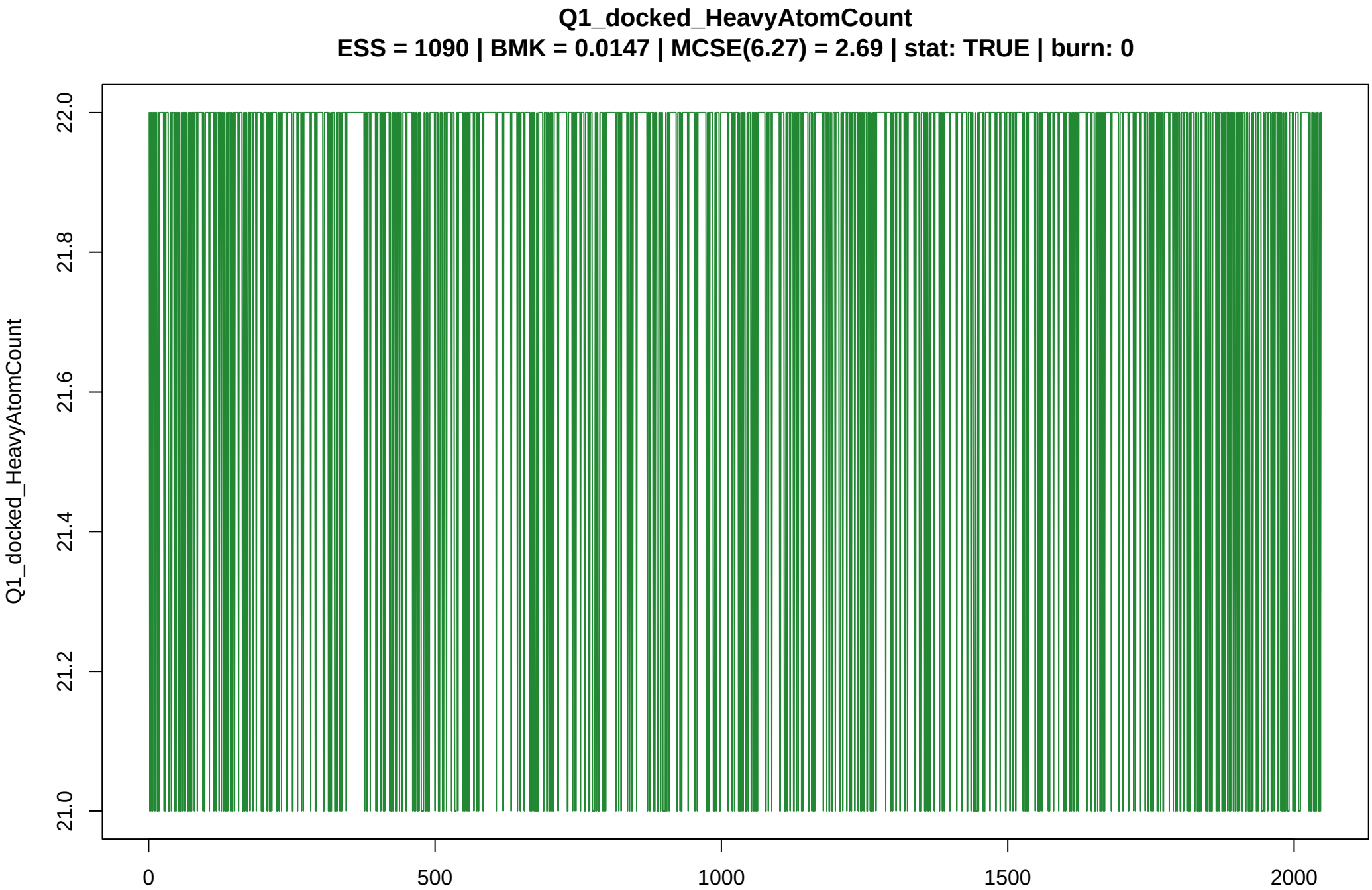

IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 1632
IQR_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

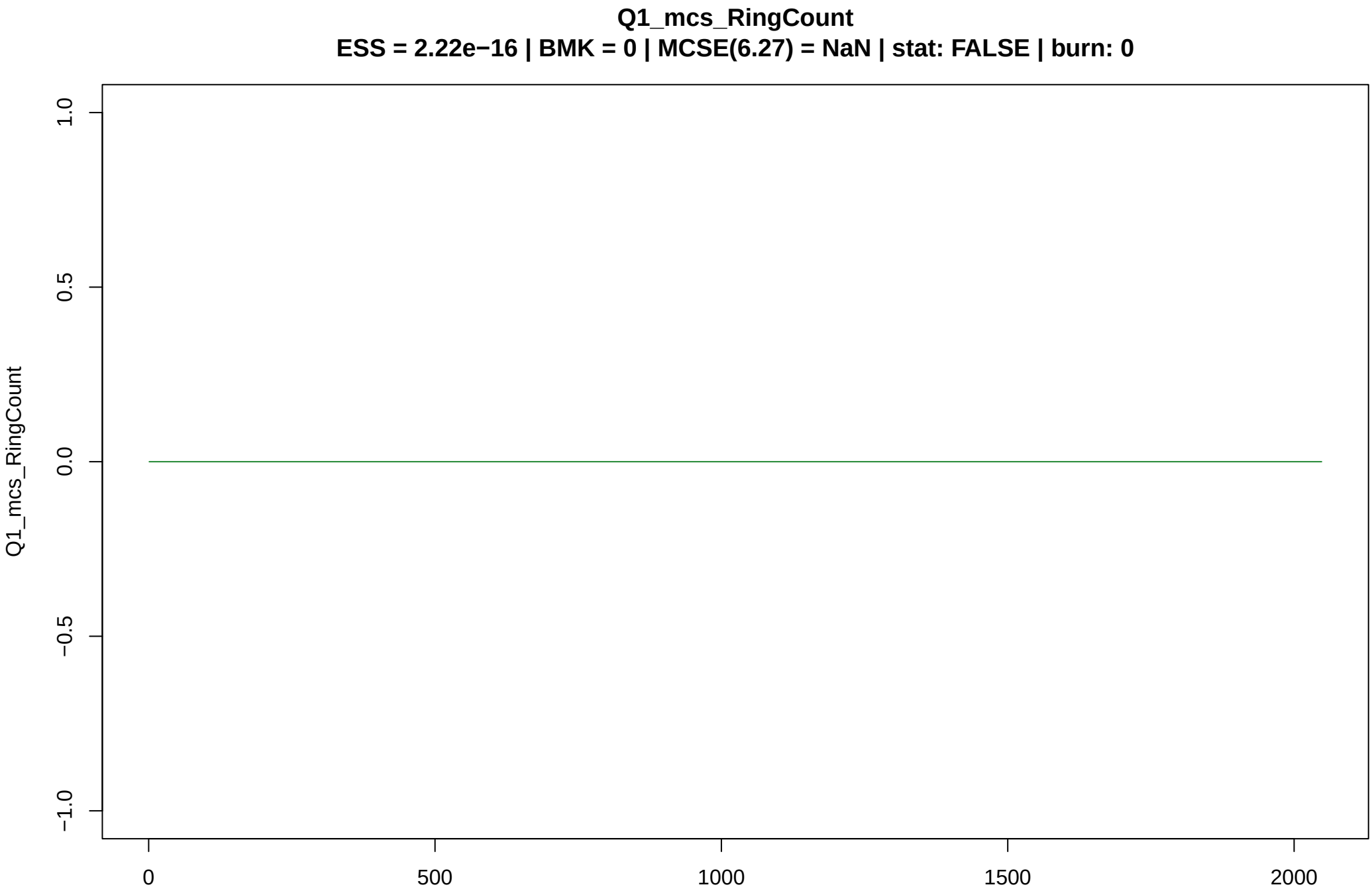

IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632
IQR_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

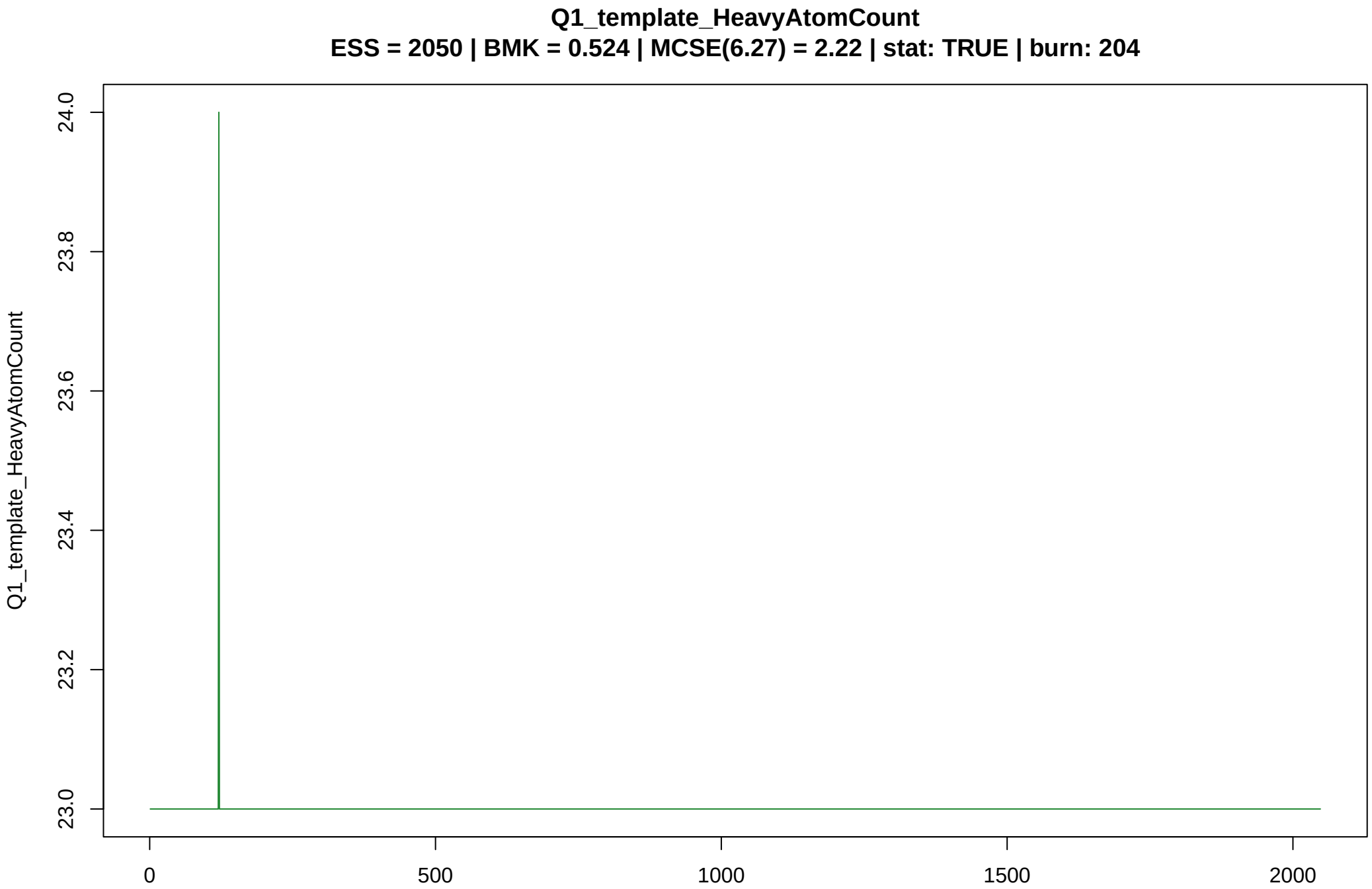

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

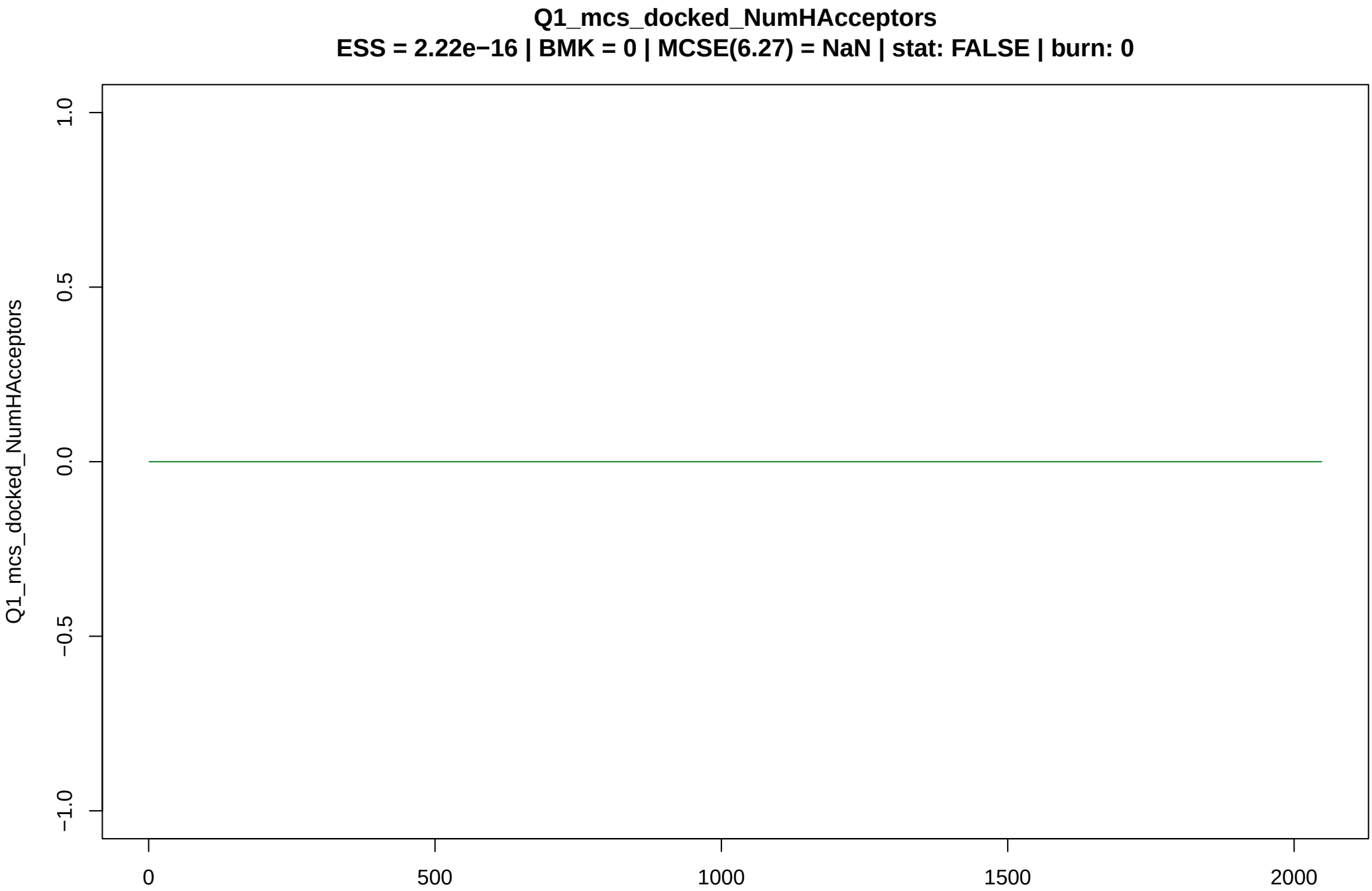

Q1_log_RMSD
ESS = 1580 | BMK = 0.0486 | MCSE(6.27) = 2.42 | stat: FALSE | burn: 0
Q1_log_RMSD
0.86
0.88
0.90
0.92
0.94
0.96
0
500
1000
1500
2000

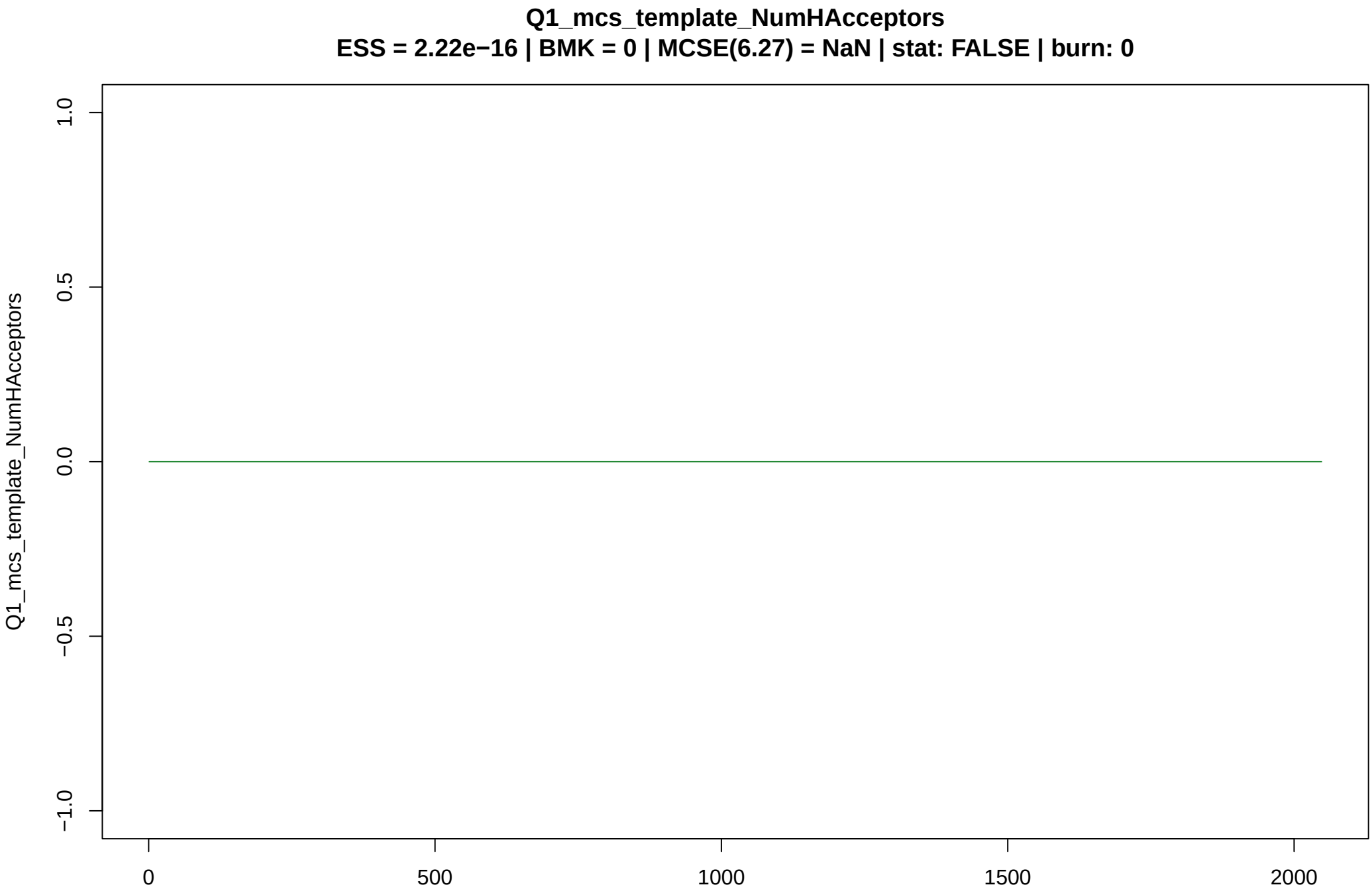

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1430 | BMK = 0.06 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

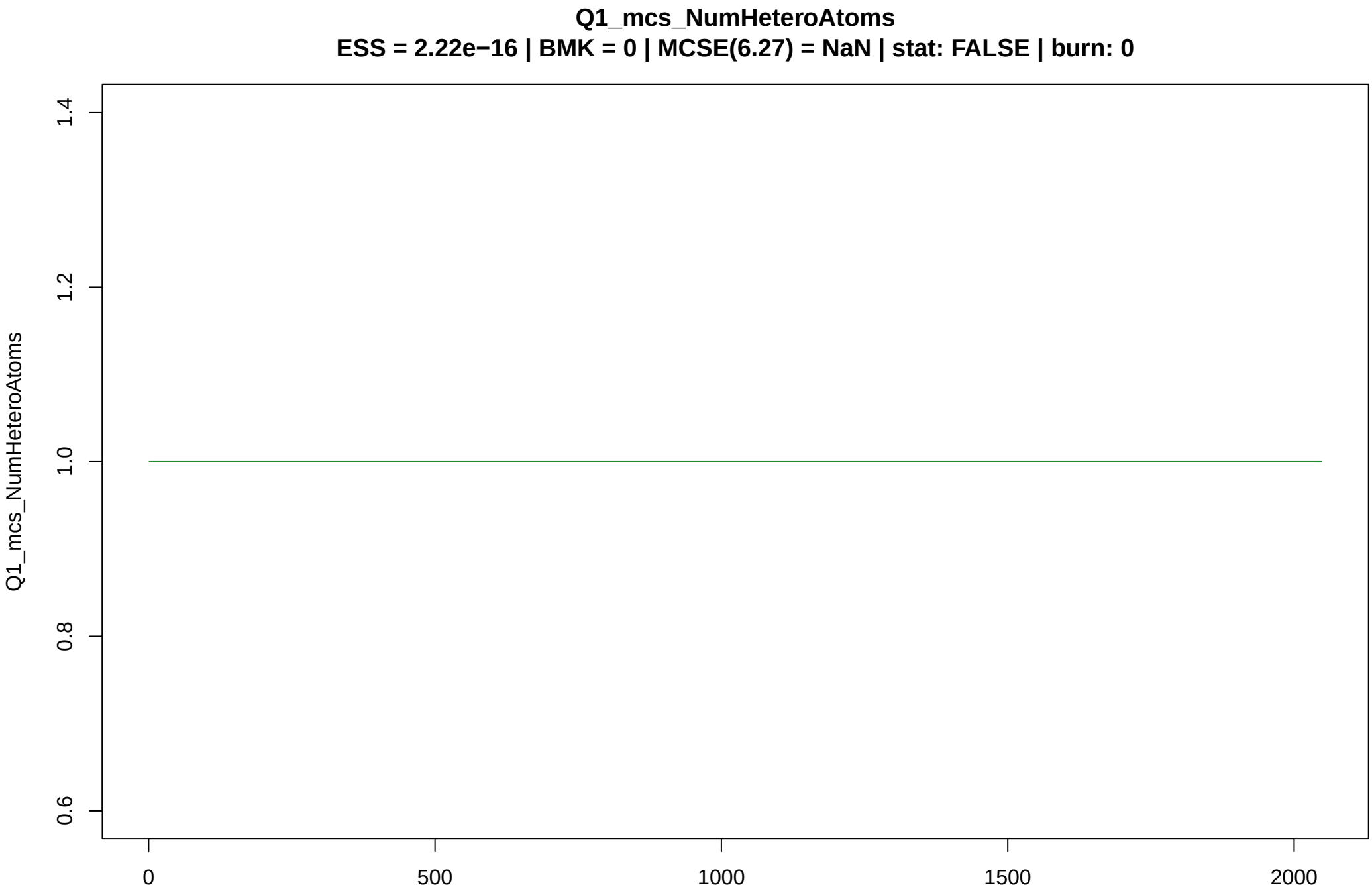

Q1_docked_HeavyAtomCount
ESS = 1090 | BMK = 0.0147 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

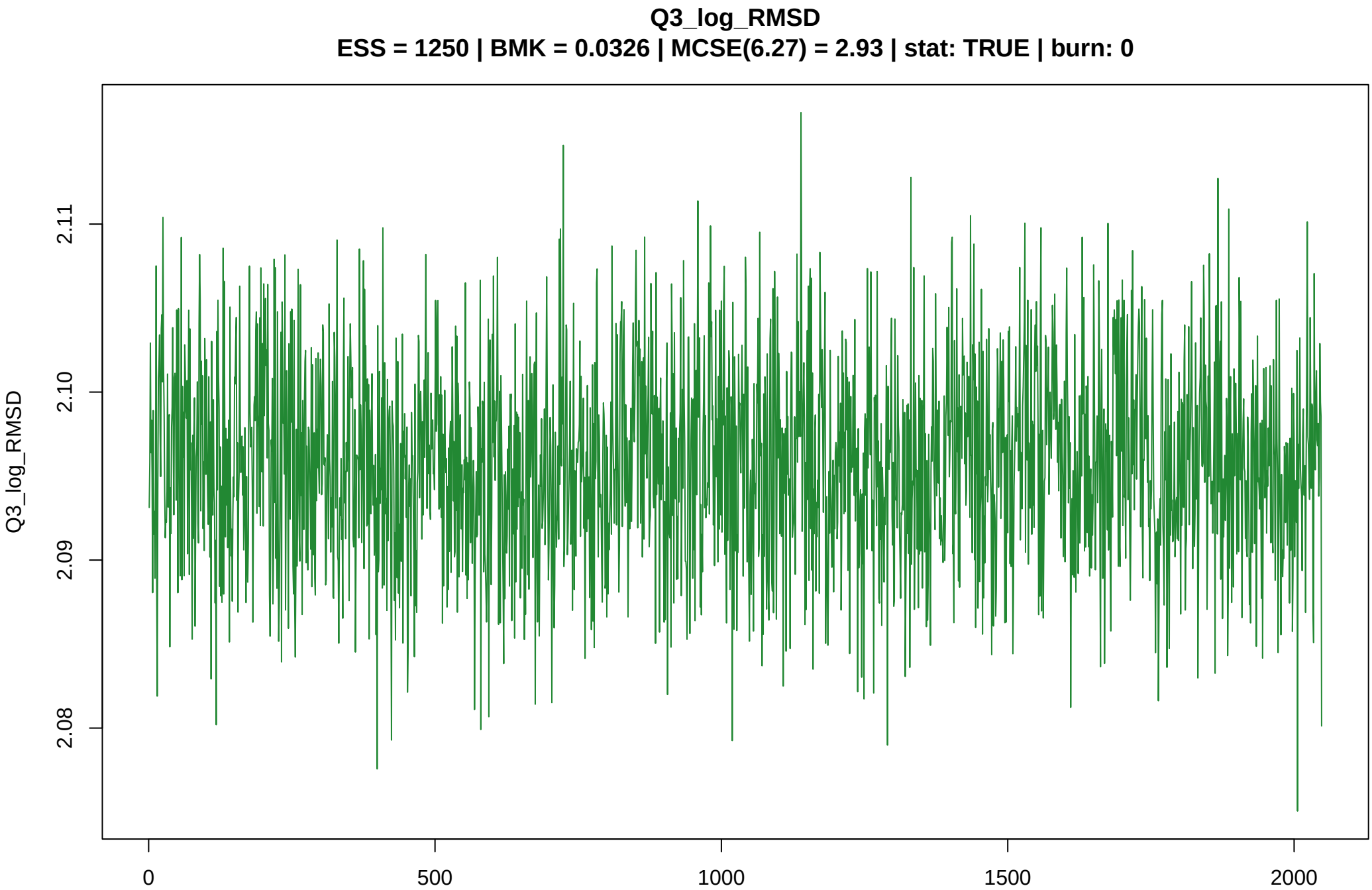

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

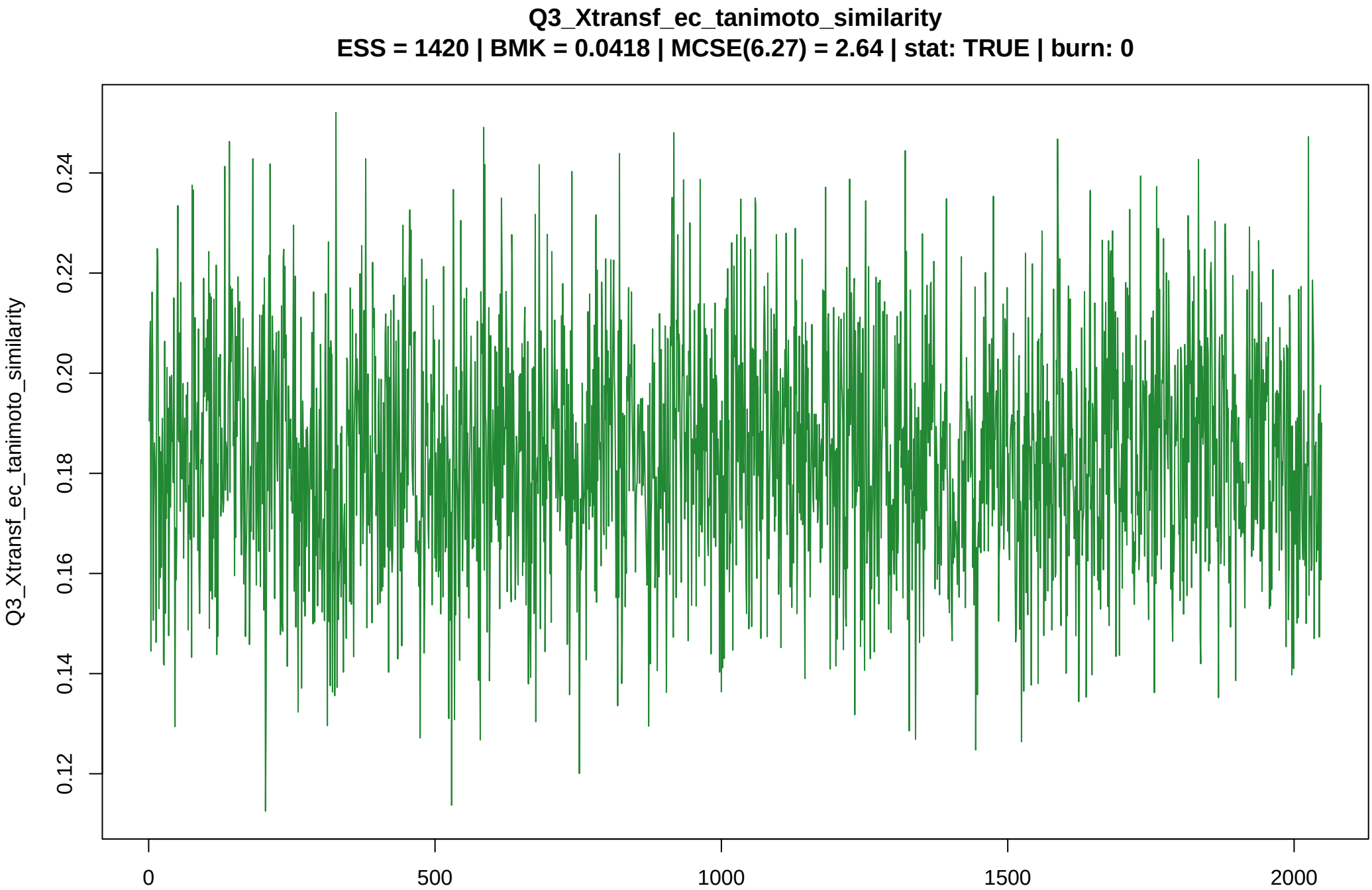

Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.524 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204
Q1_template_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

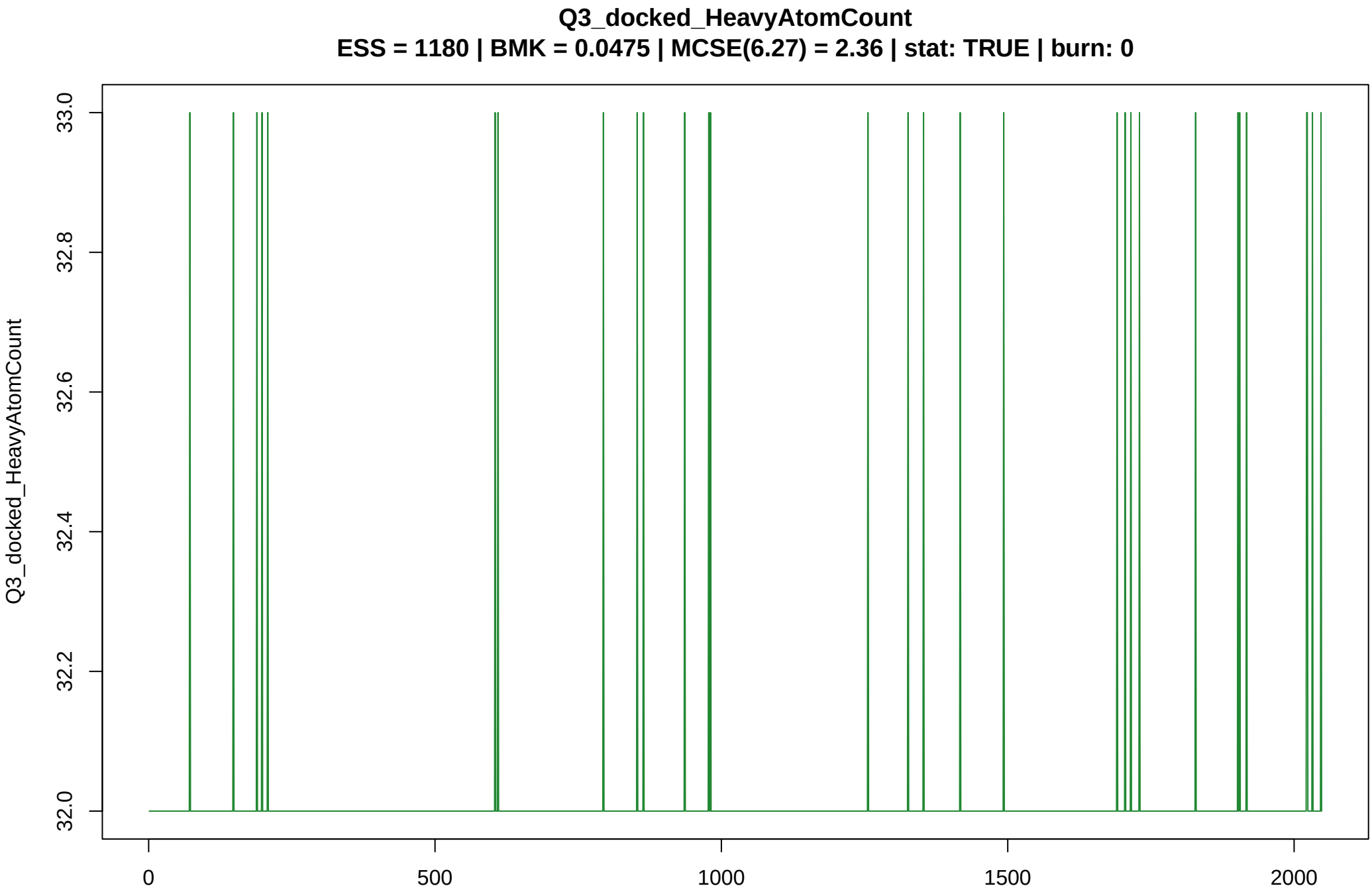

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

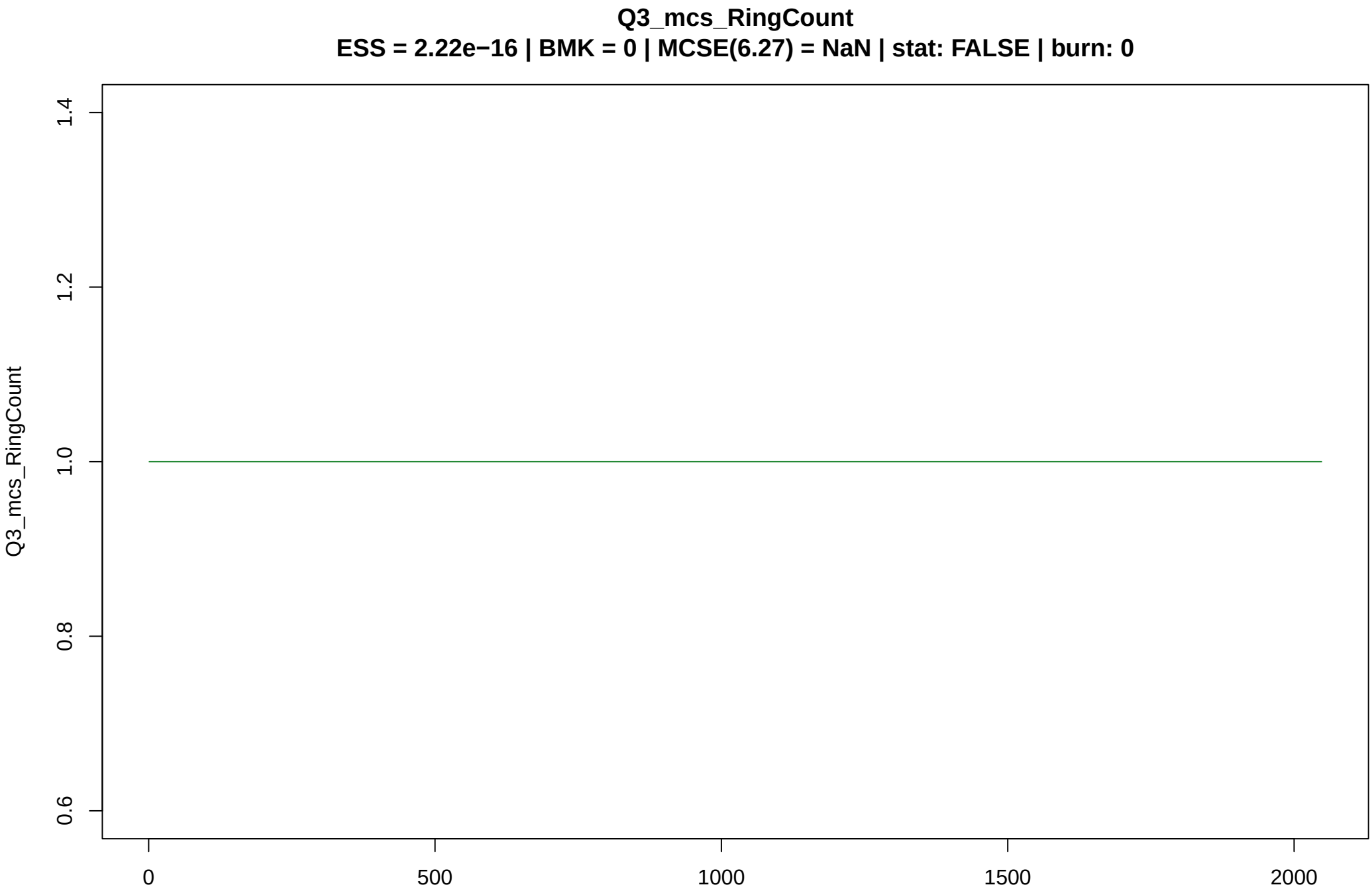

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

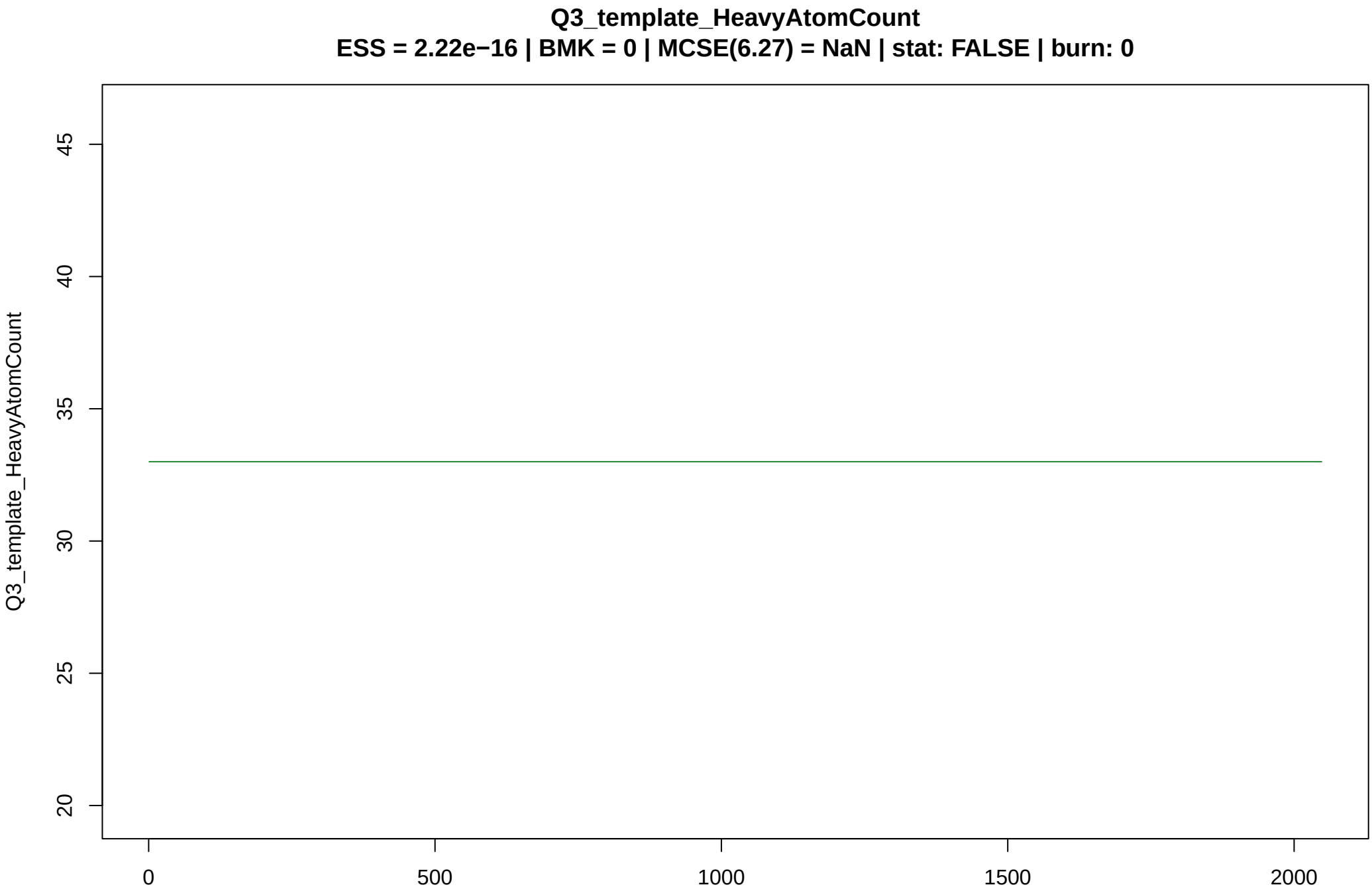

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

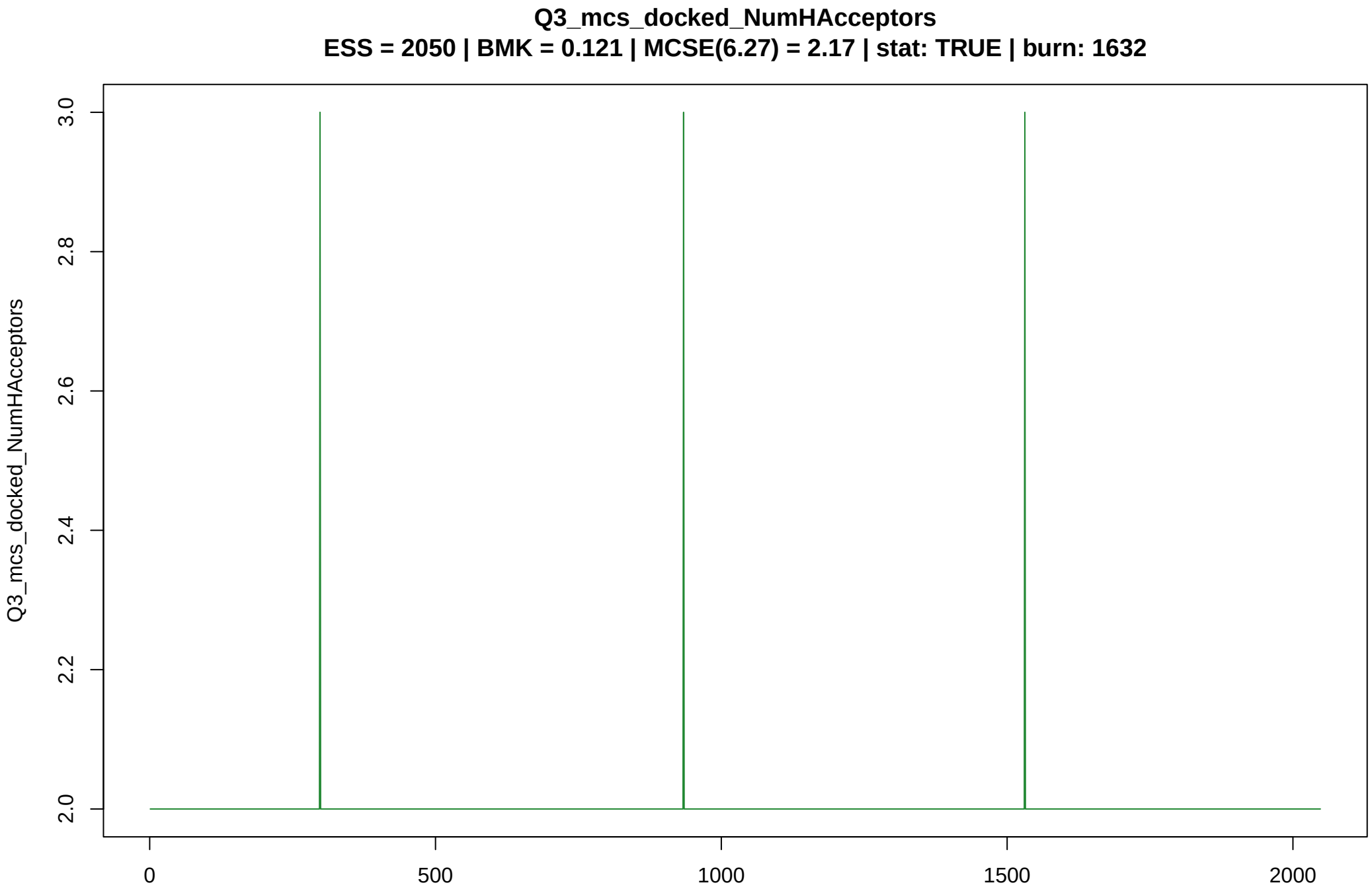

Q3_log_RMSD
ESS = 1250 | BMK = 0.0326 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

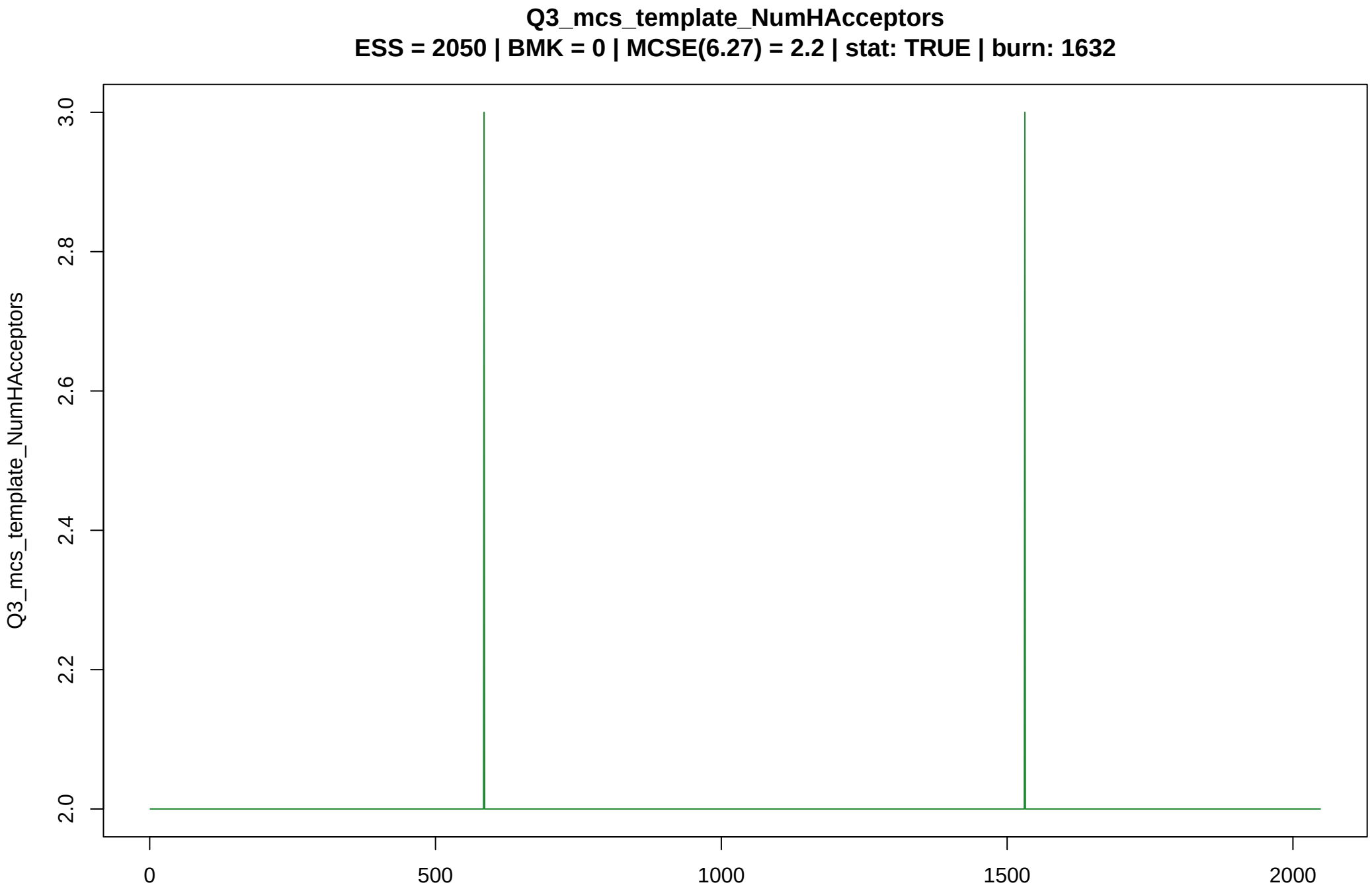

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1420 | BMK = 0.0418 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.12
0.14
0.16
0.18
0.20
0.22
0.24
0
500
1000
1500
2000

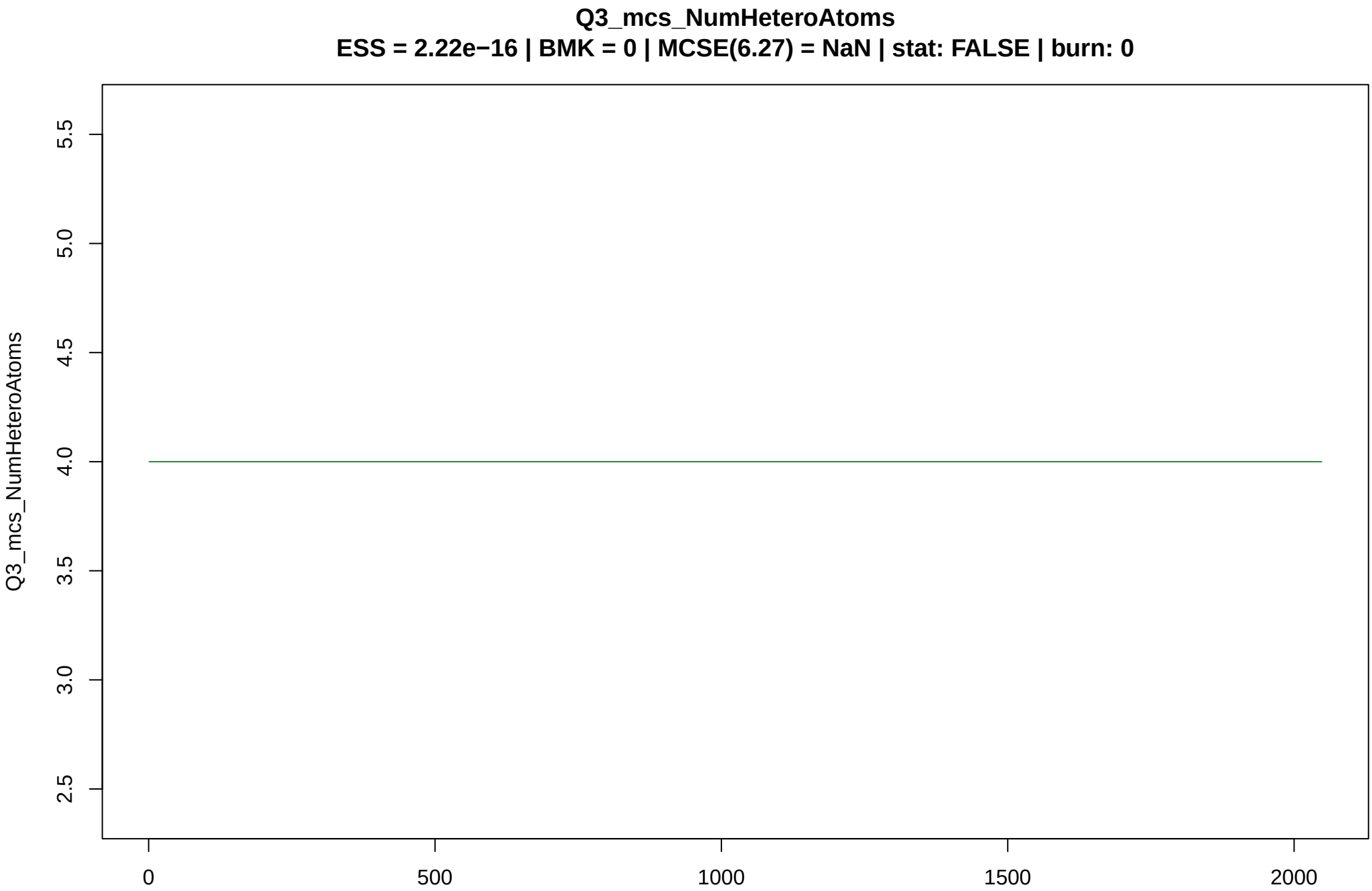

Q3_docked_HeavyAtomCount
ESS = 1180 | BMK = 0.0475 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

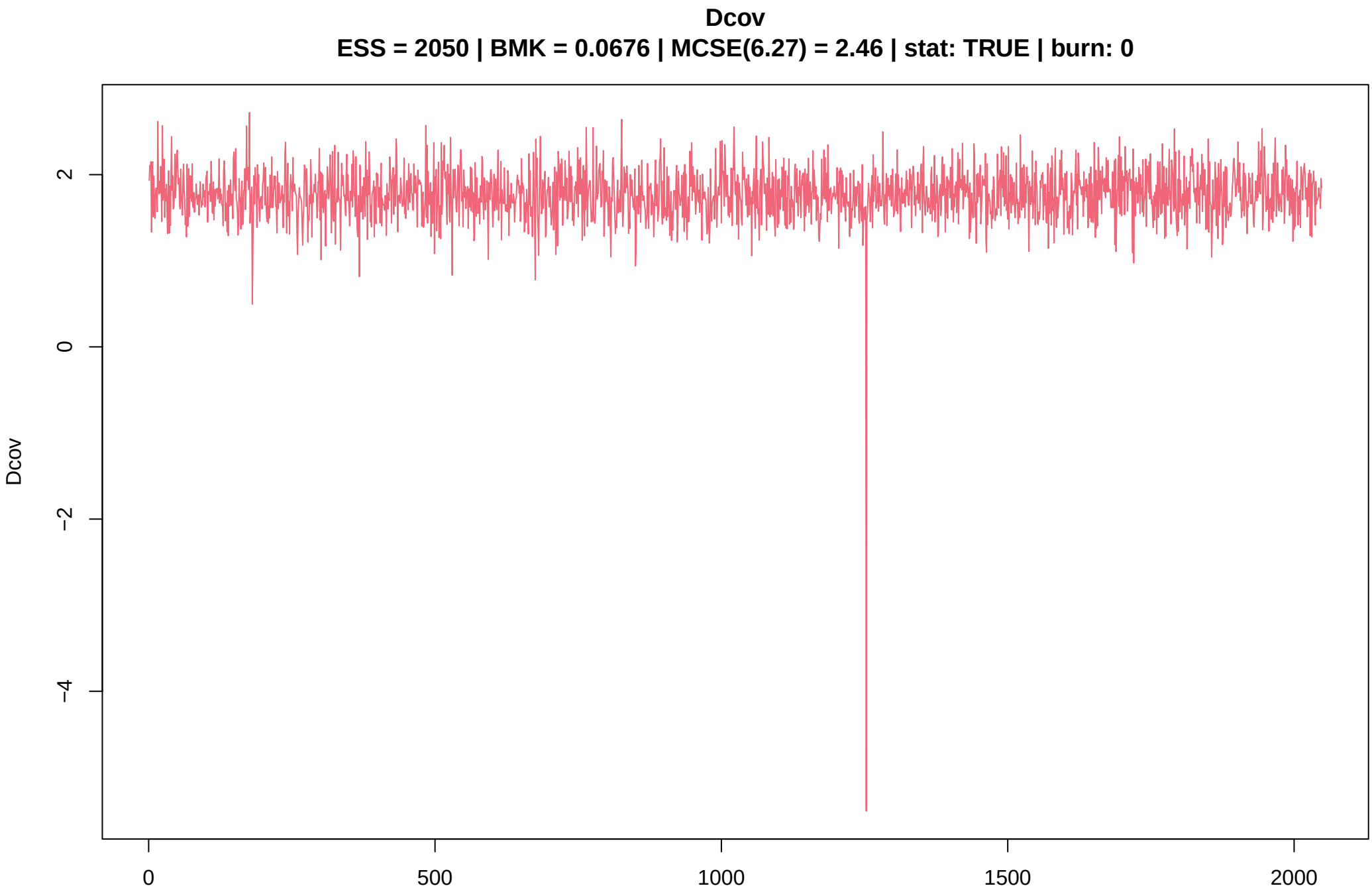

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

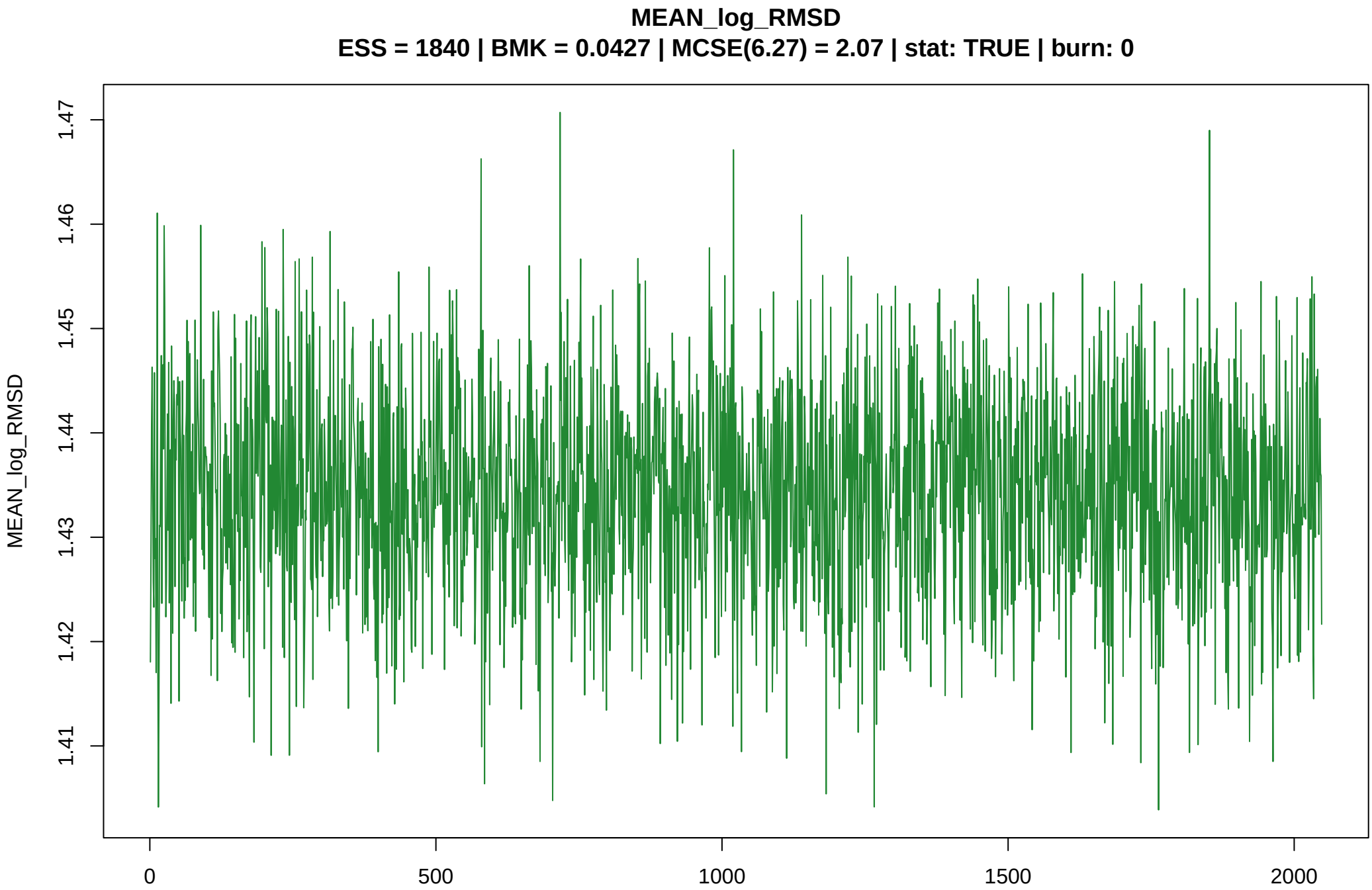

Q3_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_template_HeavyAtomCount
20
25
30
35
40
45
0
500
1000
1500
2000

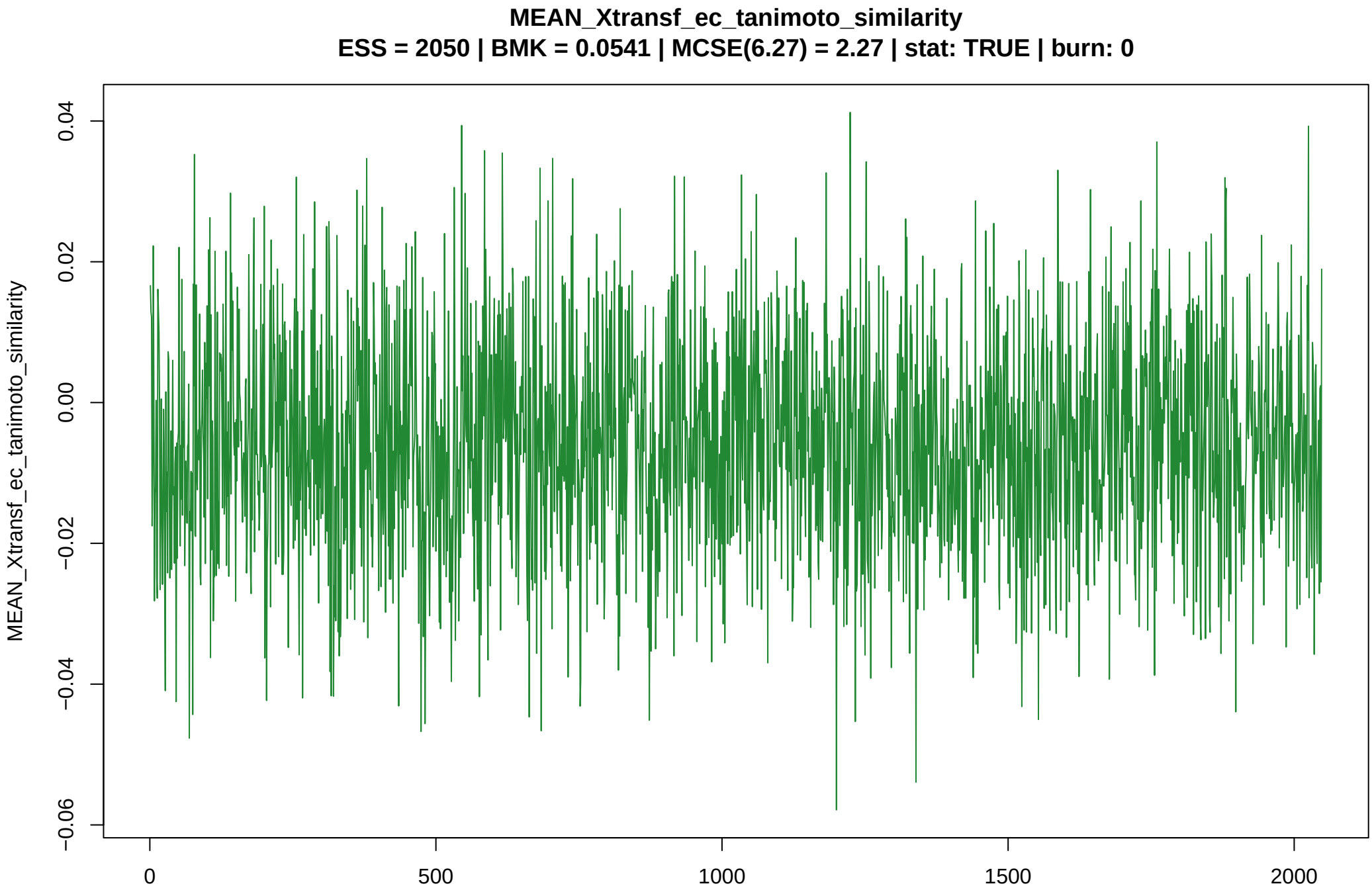

Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 1632
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

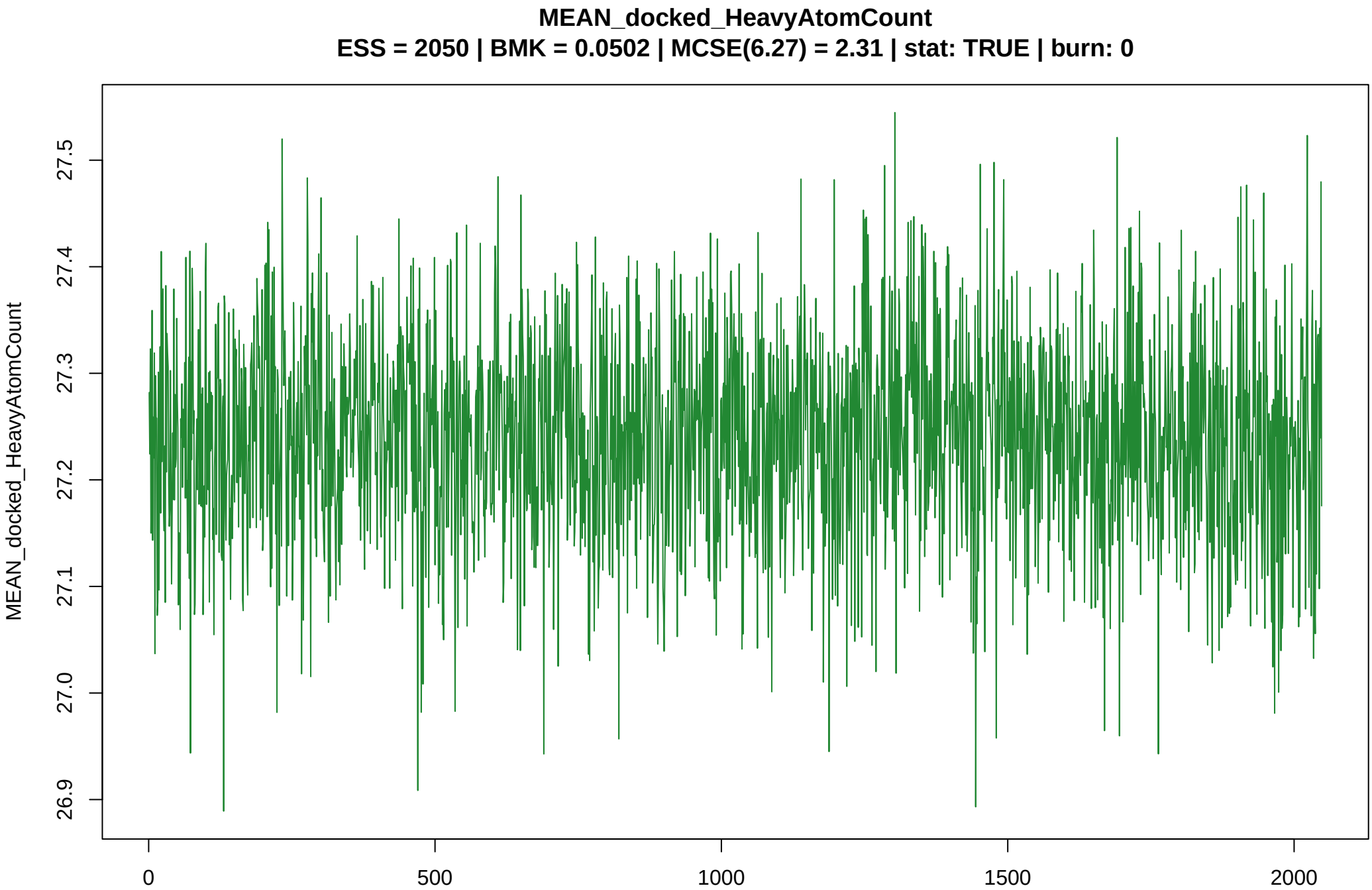

Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632
Q3_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

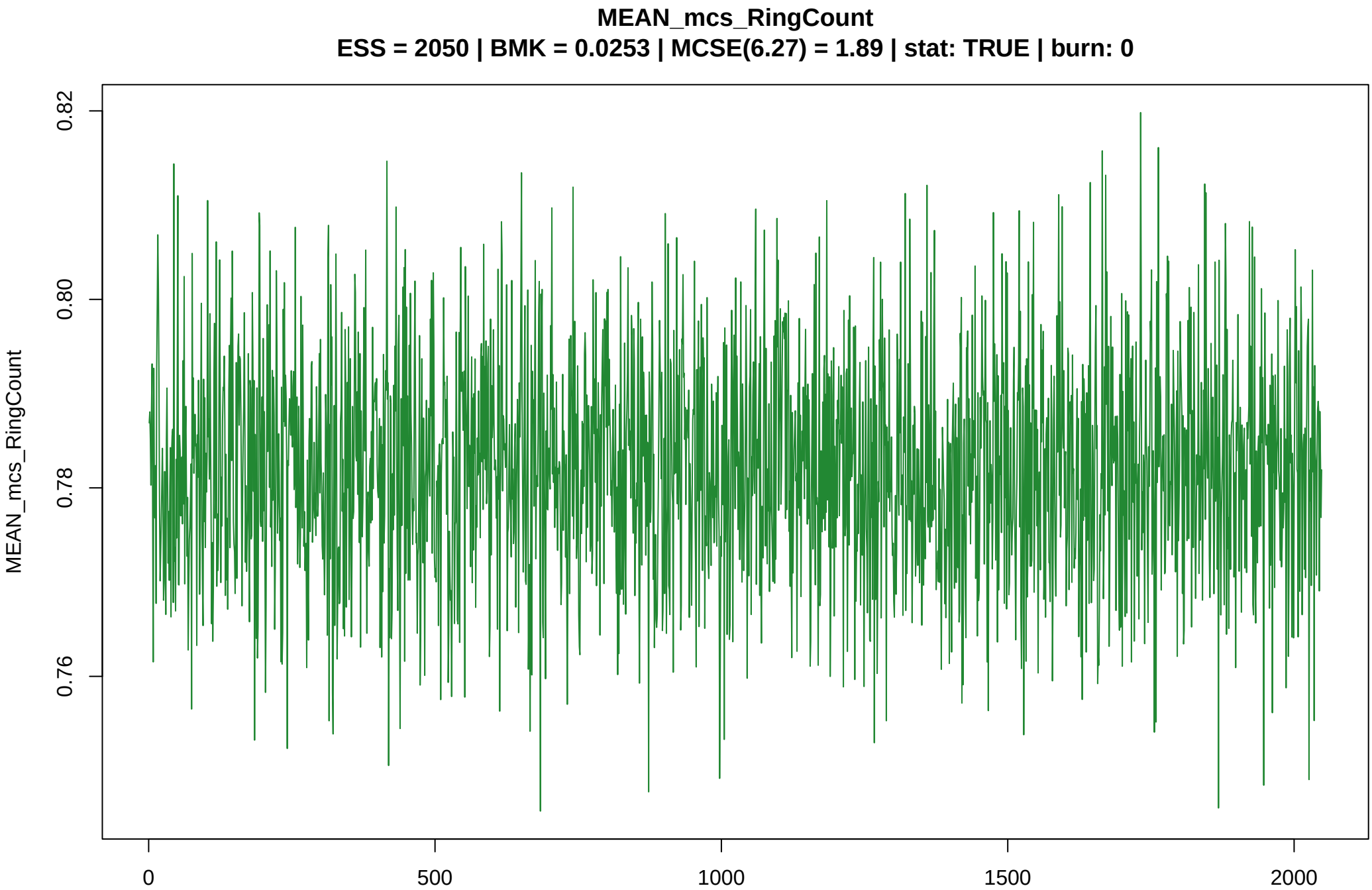

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

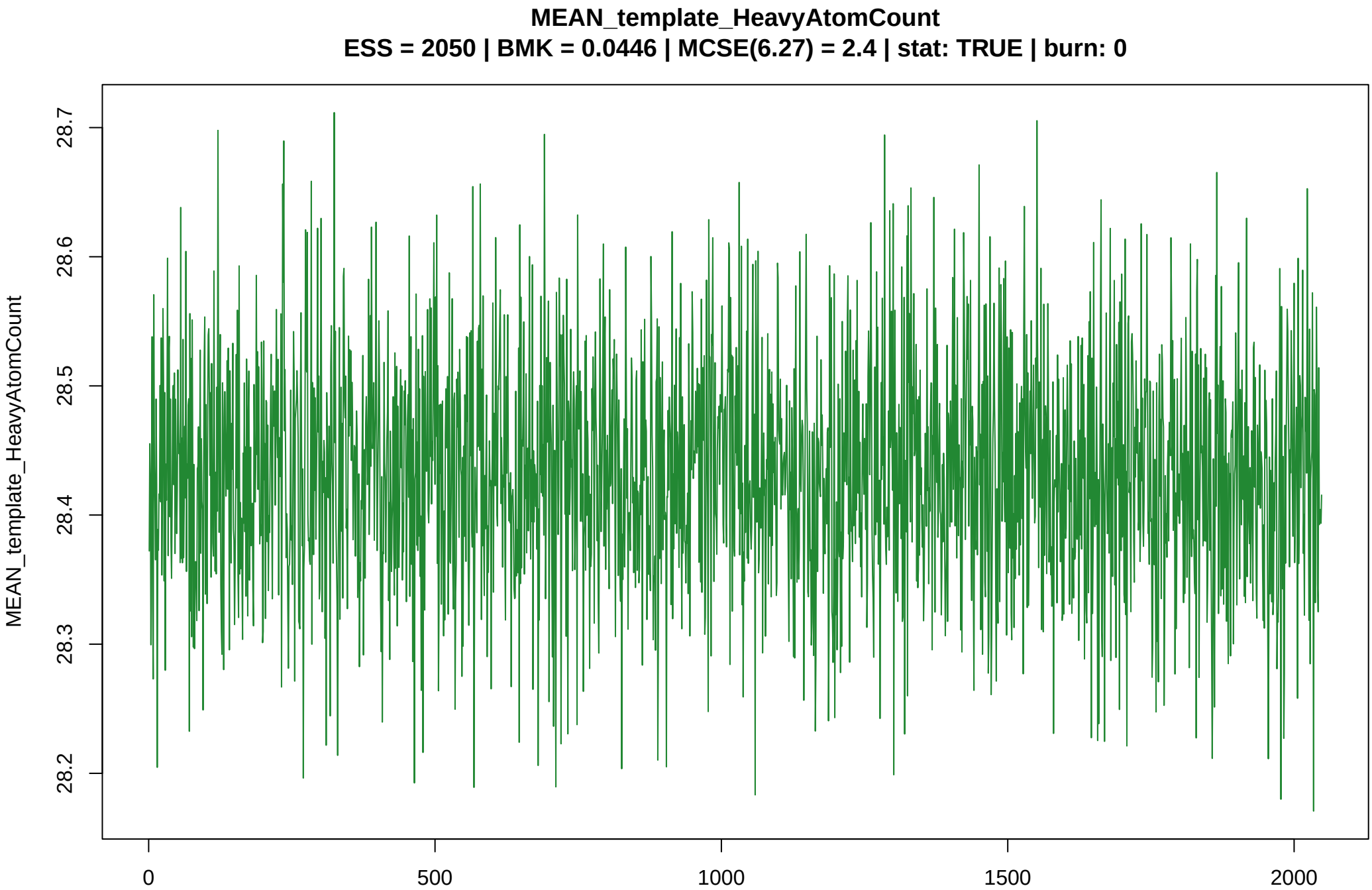

Dcov
ESS = 2050 | BMK = 0.0676 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0
Dcov
2
0
−2
−4
0
500
1000
1500
2000

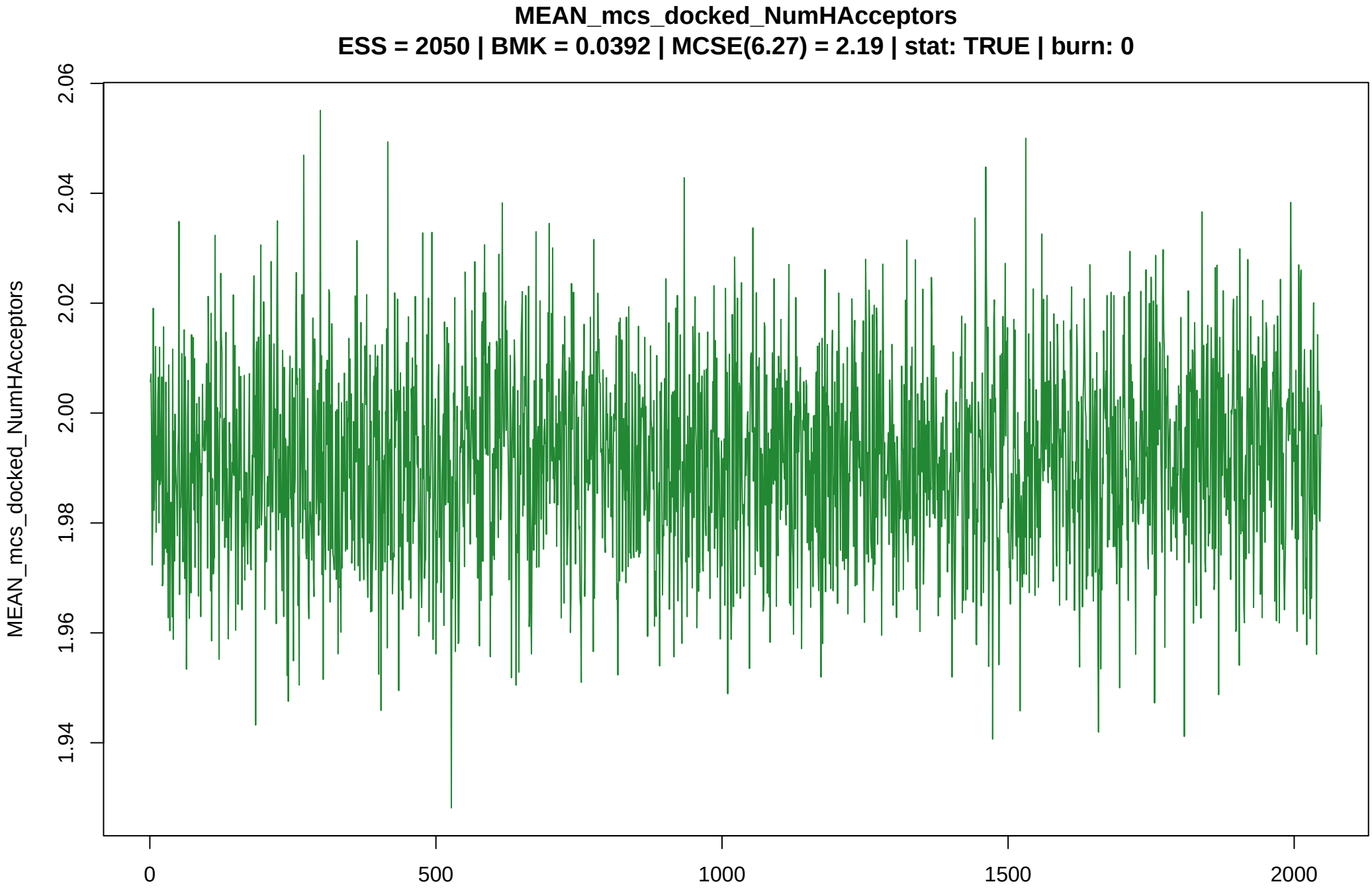

MEAN_log_RMSD
ESS = 1840 | BMK = 0.0427 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.41
1.42
1.43
1.44
1.45
1.46
1.47
0
500
1000
1500
2000

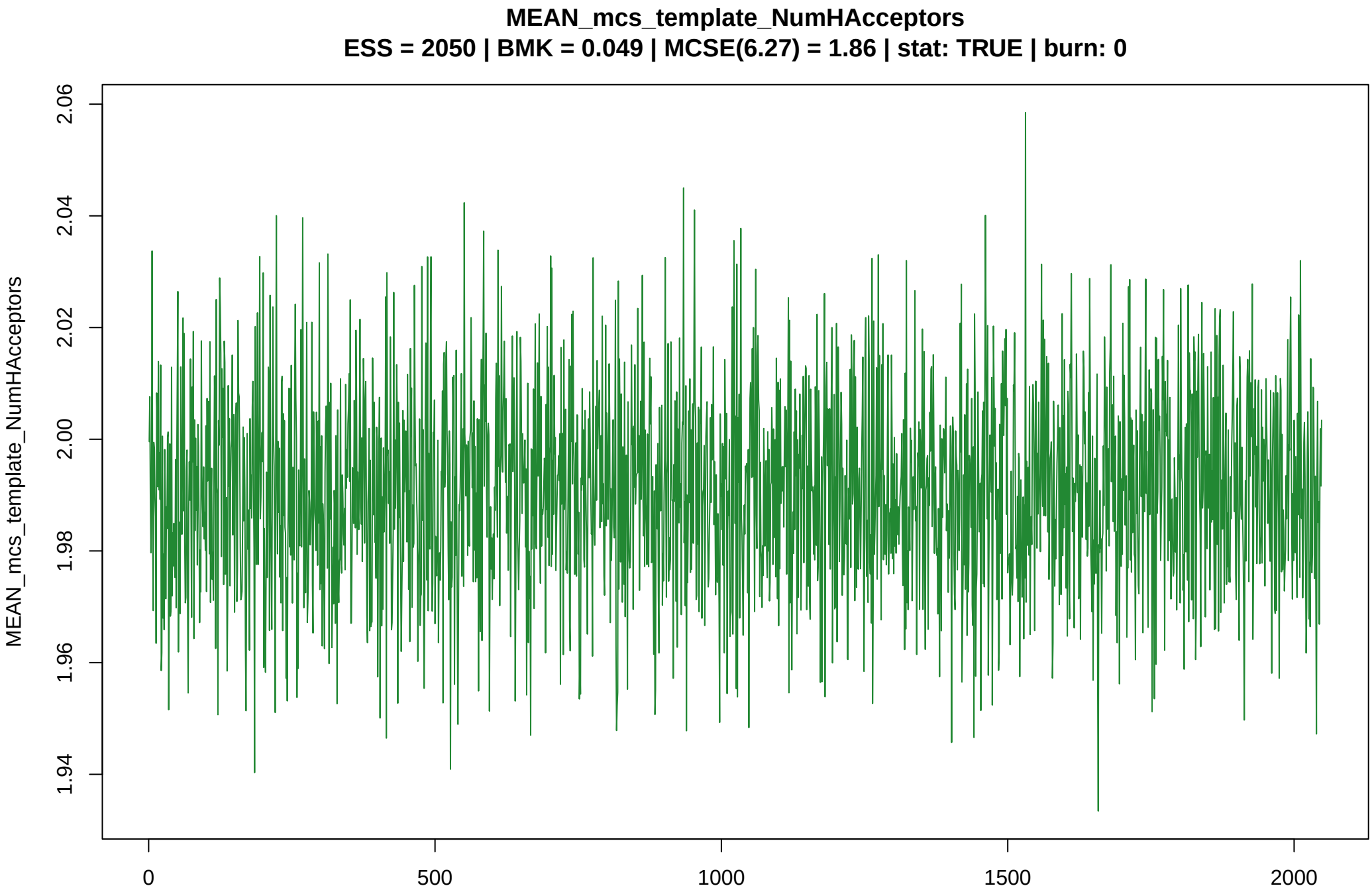

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0541 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
500
1000
1500
2000

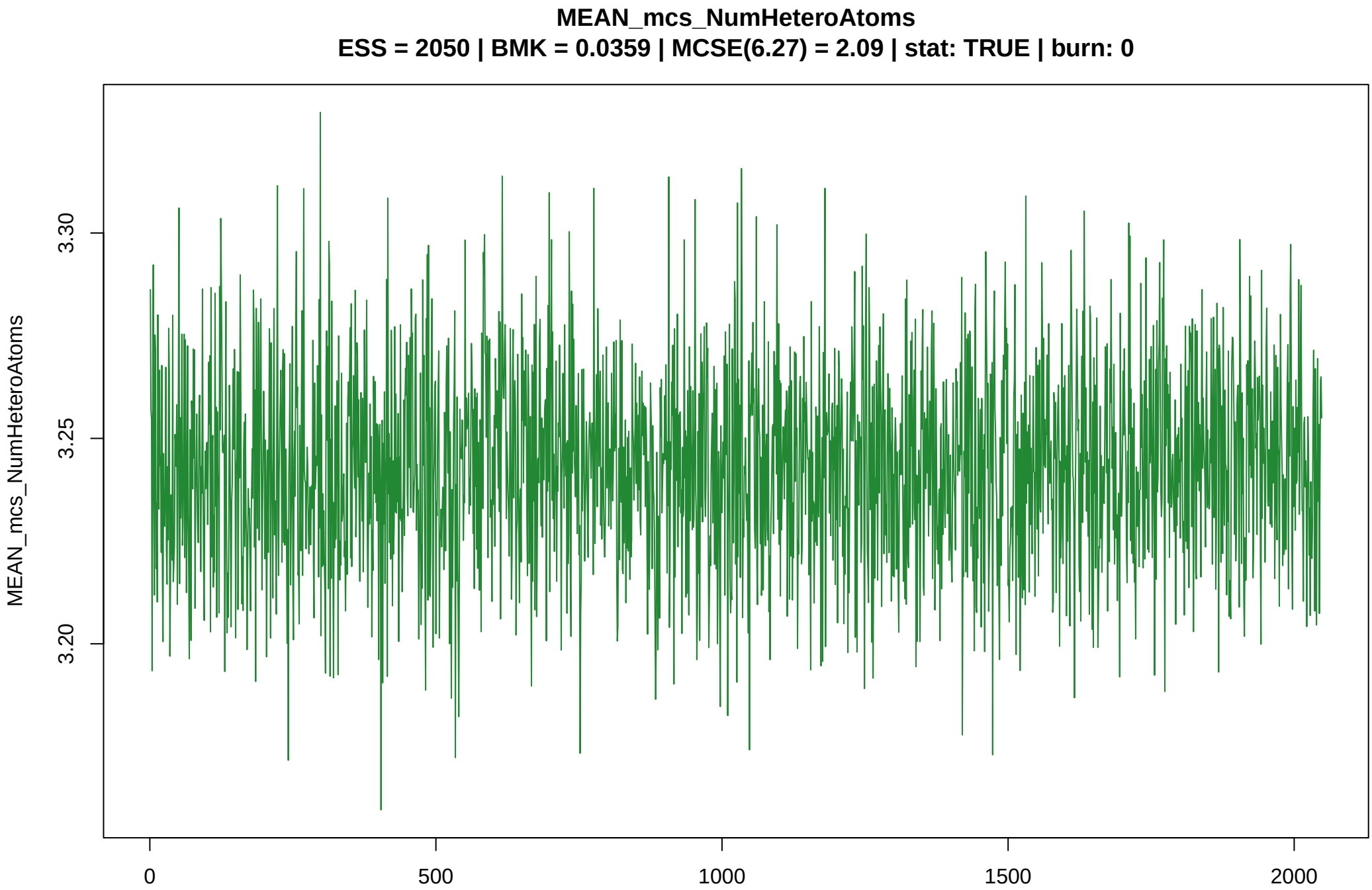

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
26.9
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

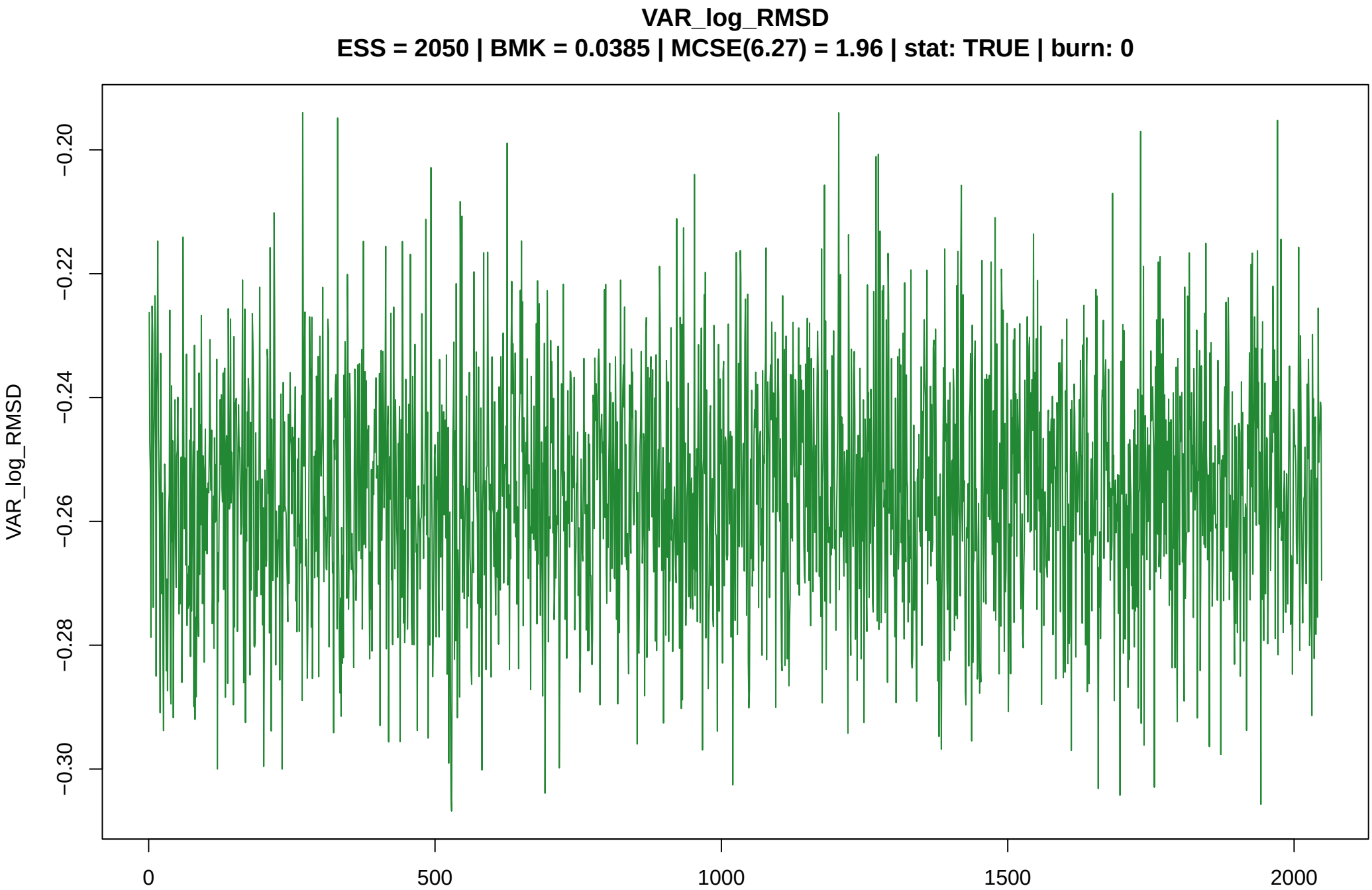

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0253 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.82
0.80
0.78
0.76
0
500
1000
1500
2000

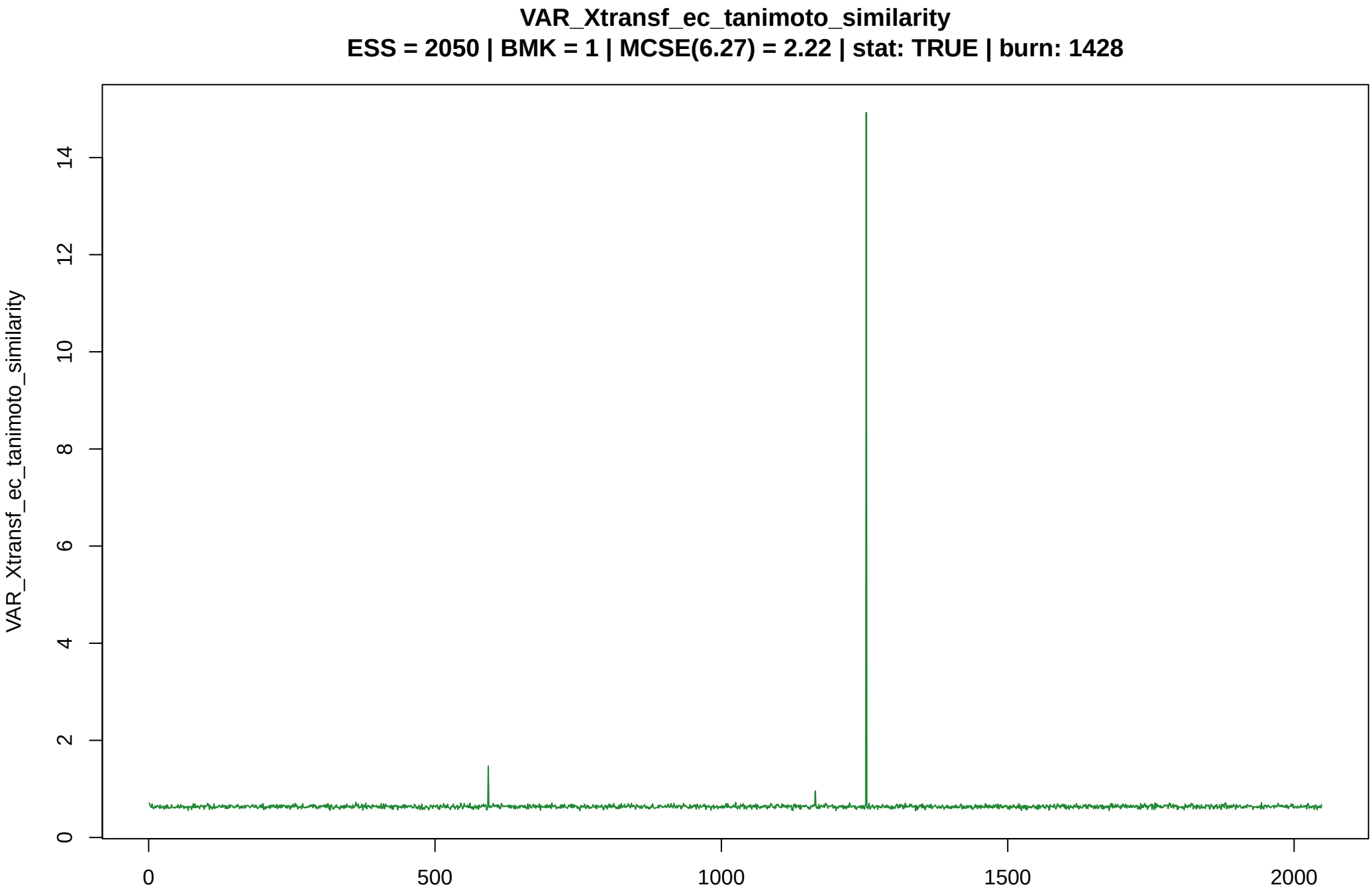

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0446 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

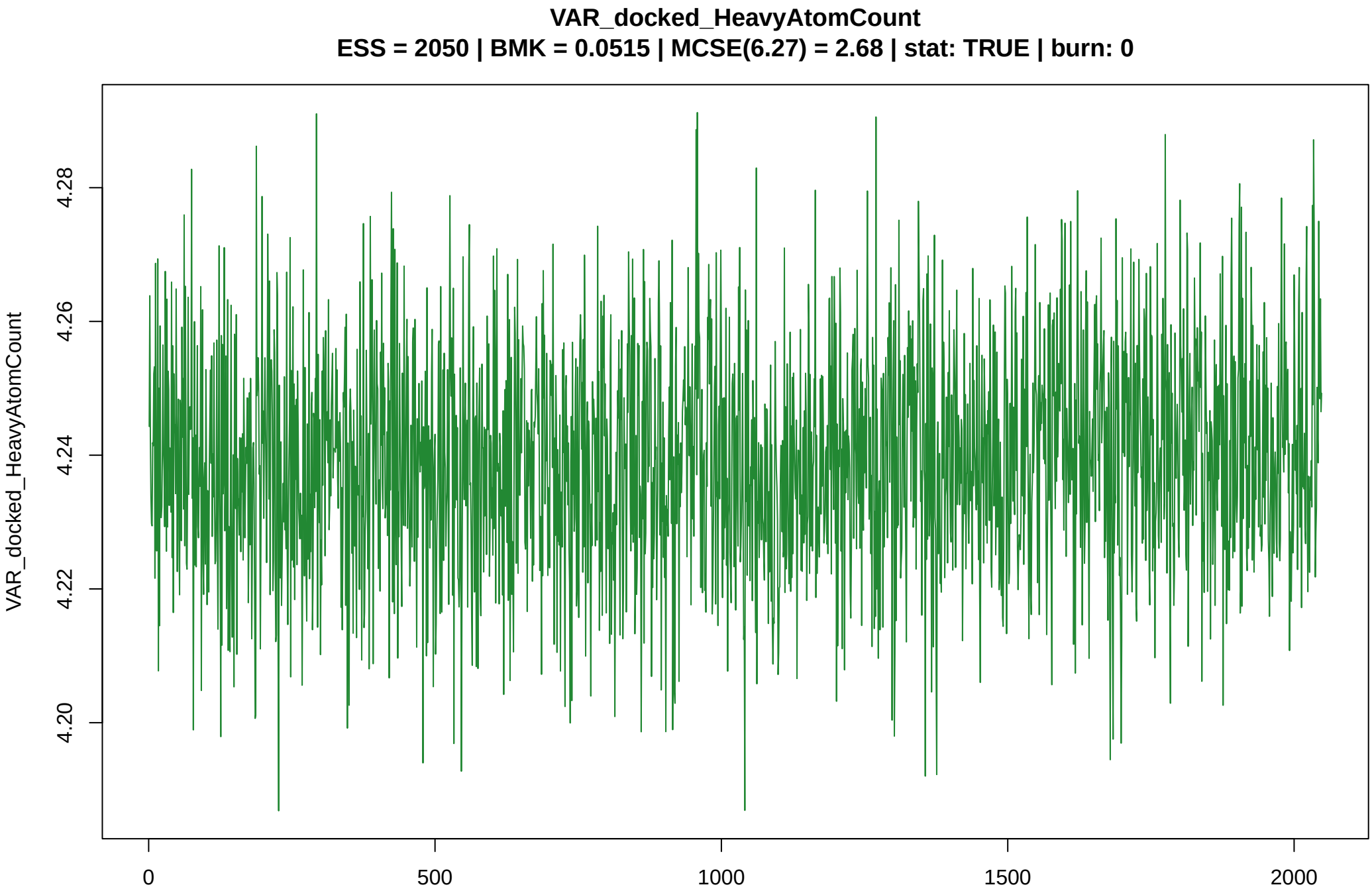

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0392 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
2.06
2.04
2.02
2.00
1.98
1.96
1.94
0
500
1000
1500
2000

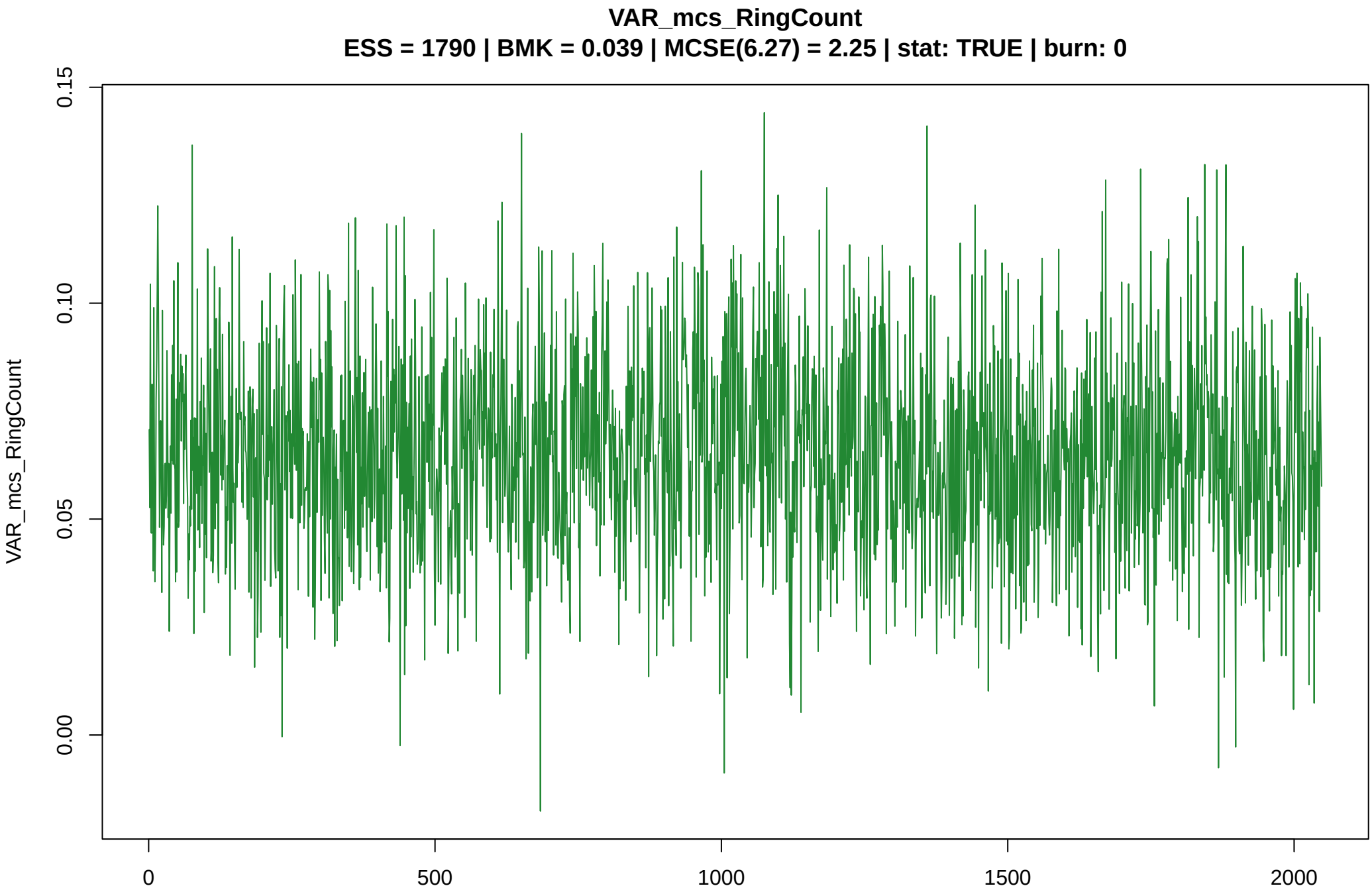

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.049 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
2.06
2.04
2.02
2.00
1.98
1.96
1.94
0
500
1000
1500
2000

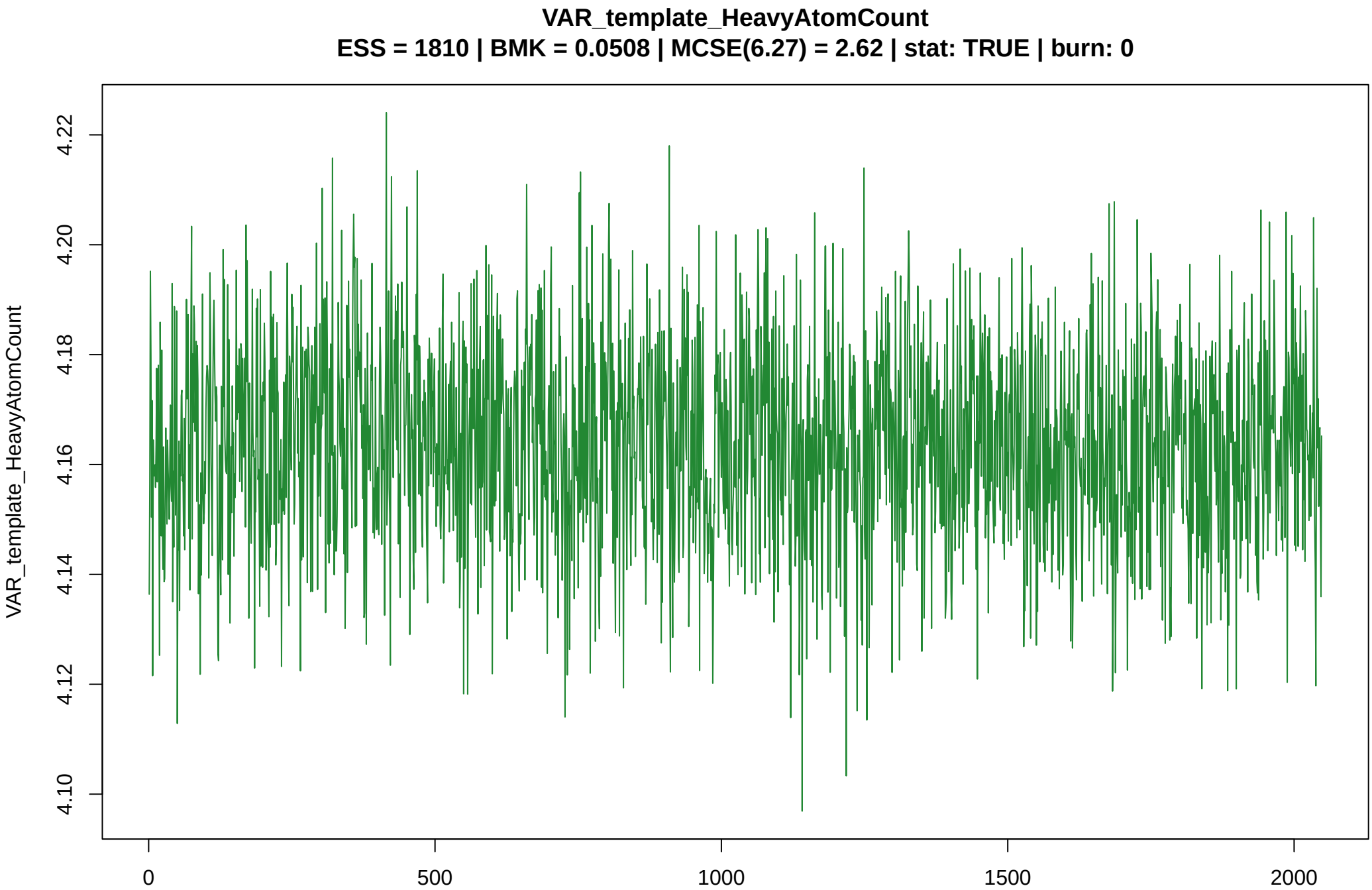

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0359 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

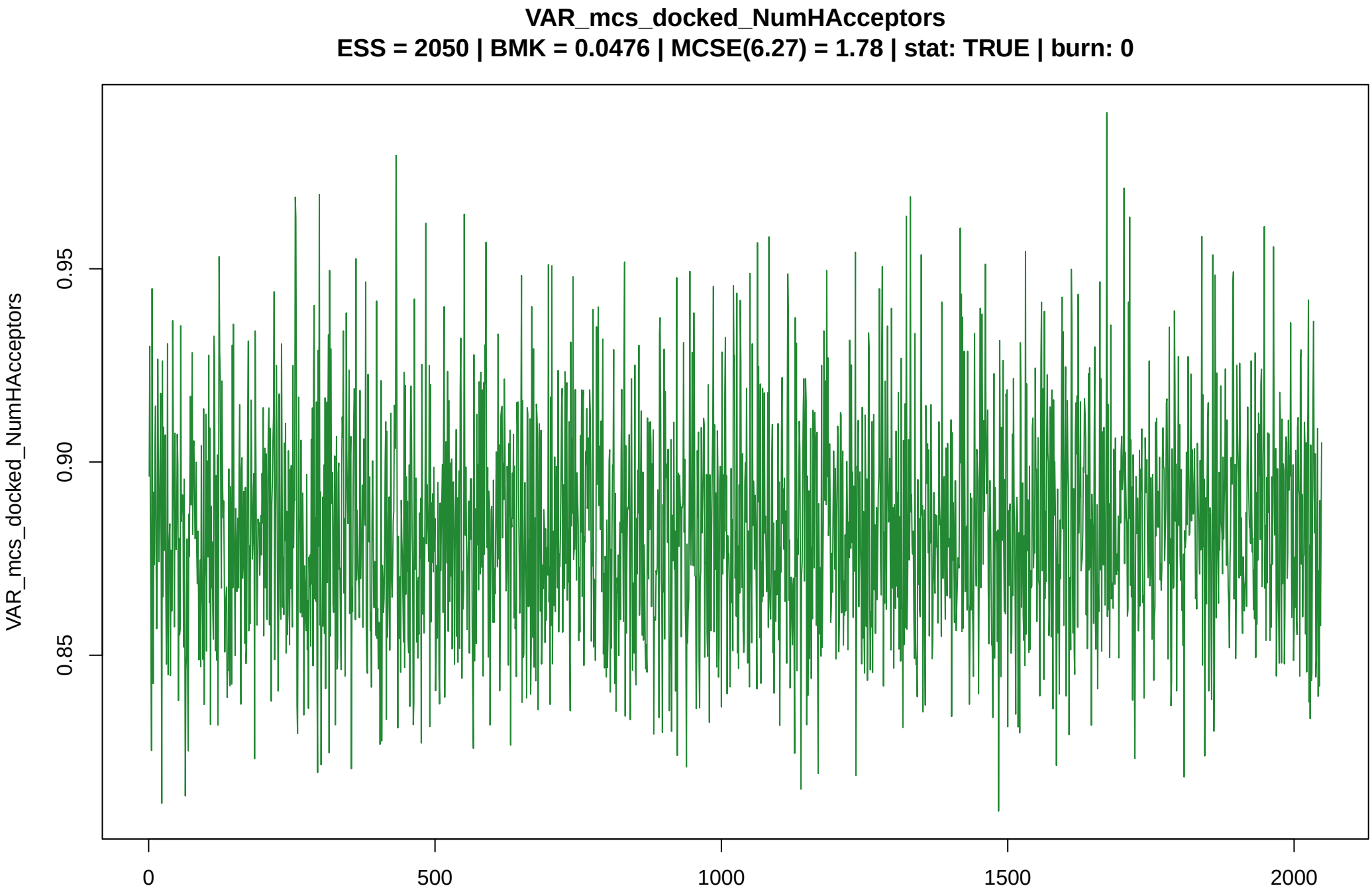

VAR_log_RMSD
ESS = 2050 | BMK = 0.0385 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0
VAR_log_RMSD
−0.20
−0.22
−0.24
−0.26
−0.28
−0.30
0
500
1000
1500
2000

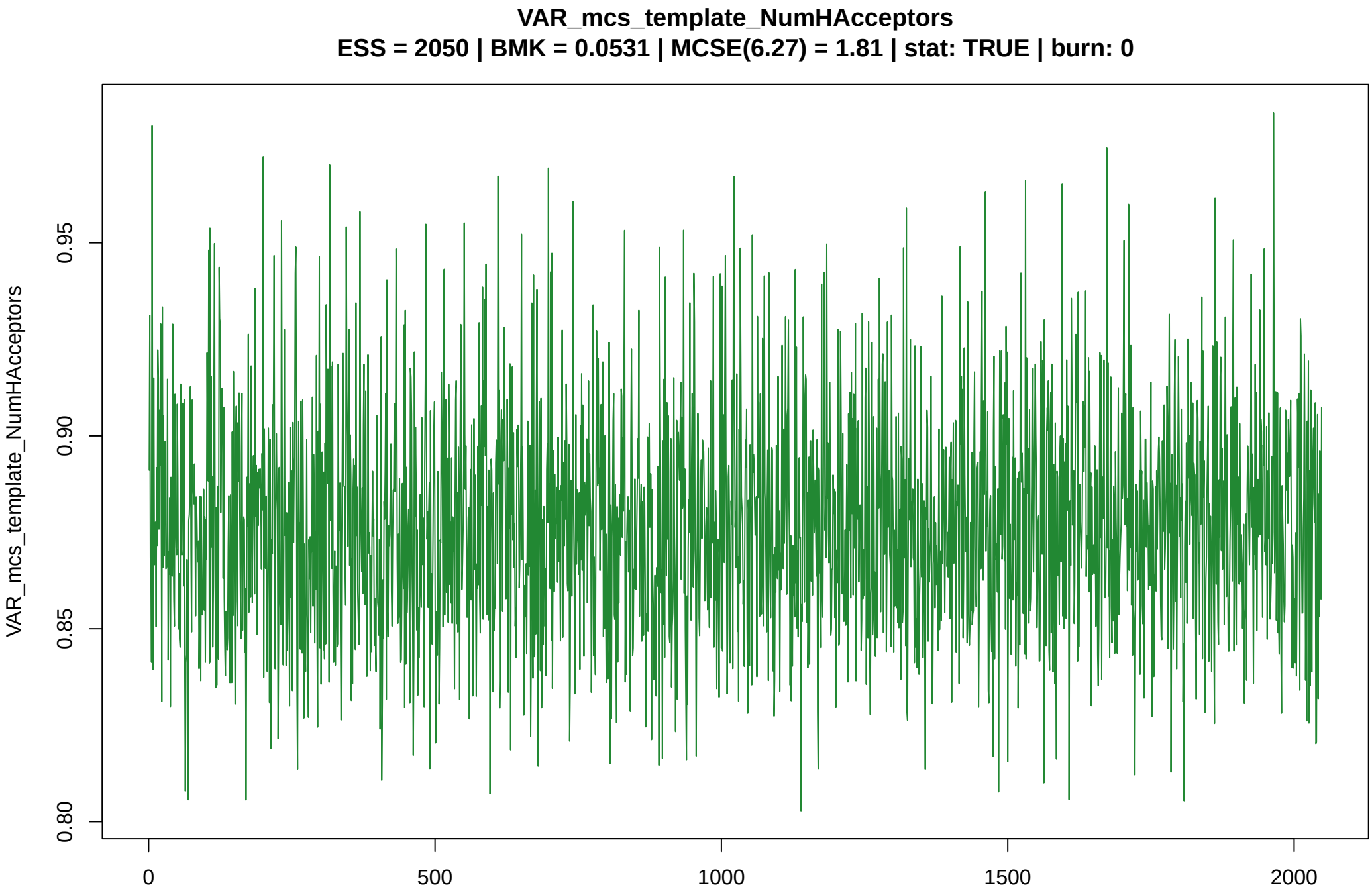

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 1 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1428
VAR_Xtransf_ec_tanimoto_similarity
0
2
4
6
8
10
12
14
0
500
1000
1500
2000

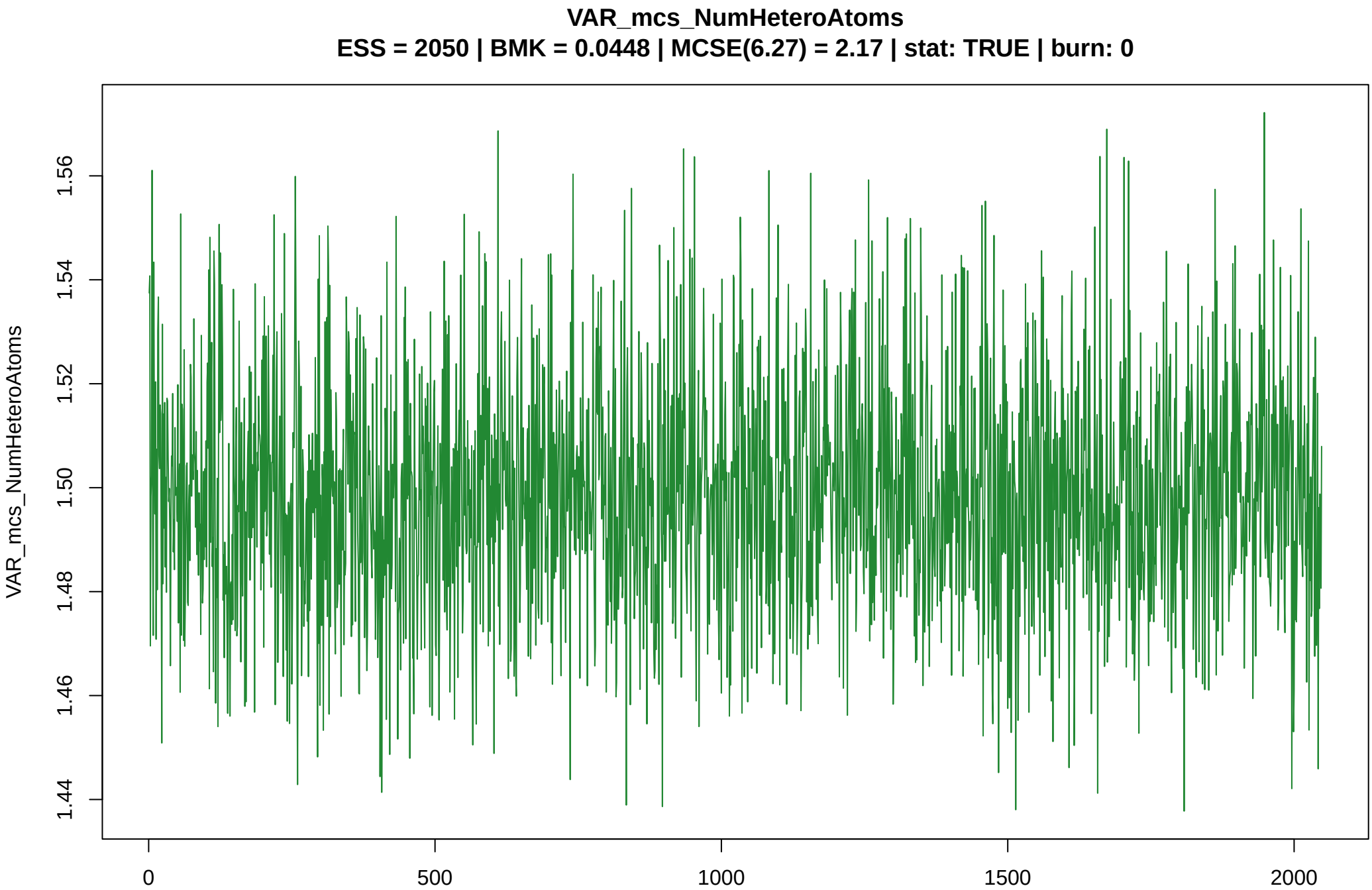

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0515 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
4.20
4.22
4.24
4.26
4.28
0
500
1000
1500
2000

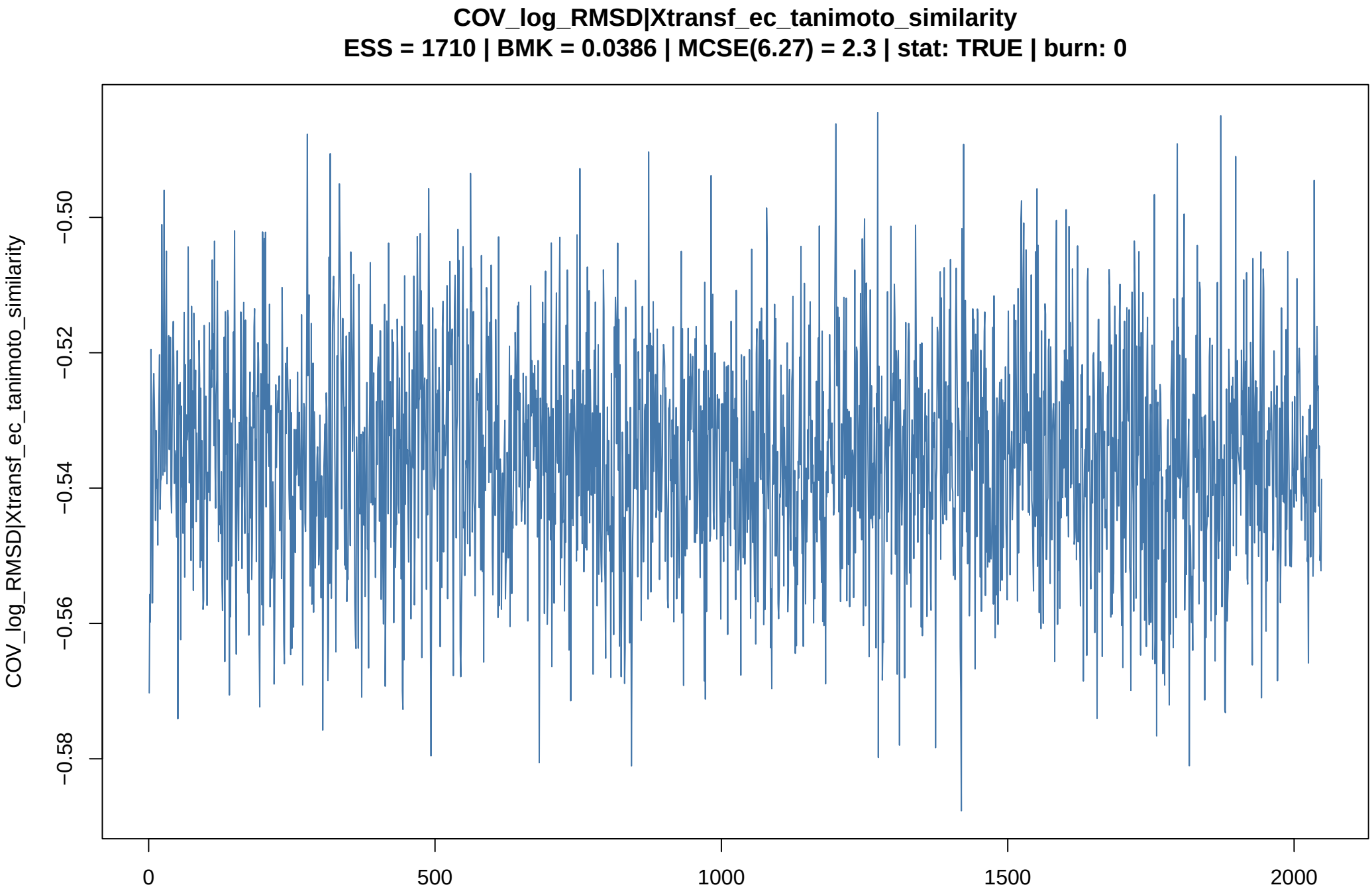

VAR_mcs_RingCount
ESS = 1790 | BMK = 0.039 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
VAR_mcs_RingCount
0.00
0.05
0.10
0.15
0
500
1000
1500
2000

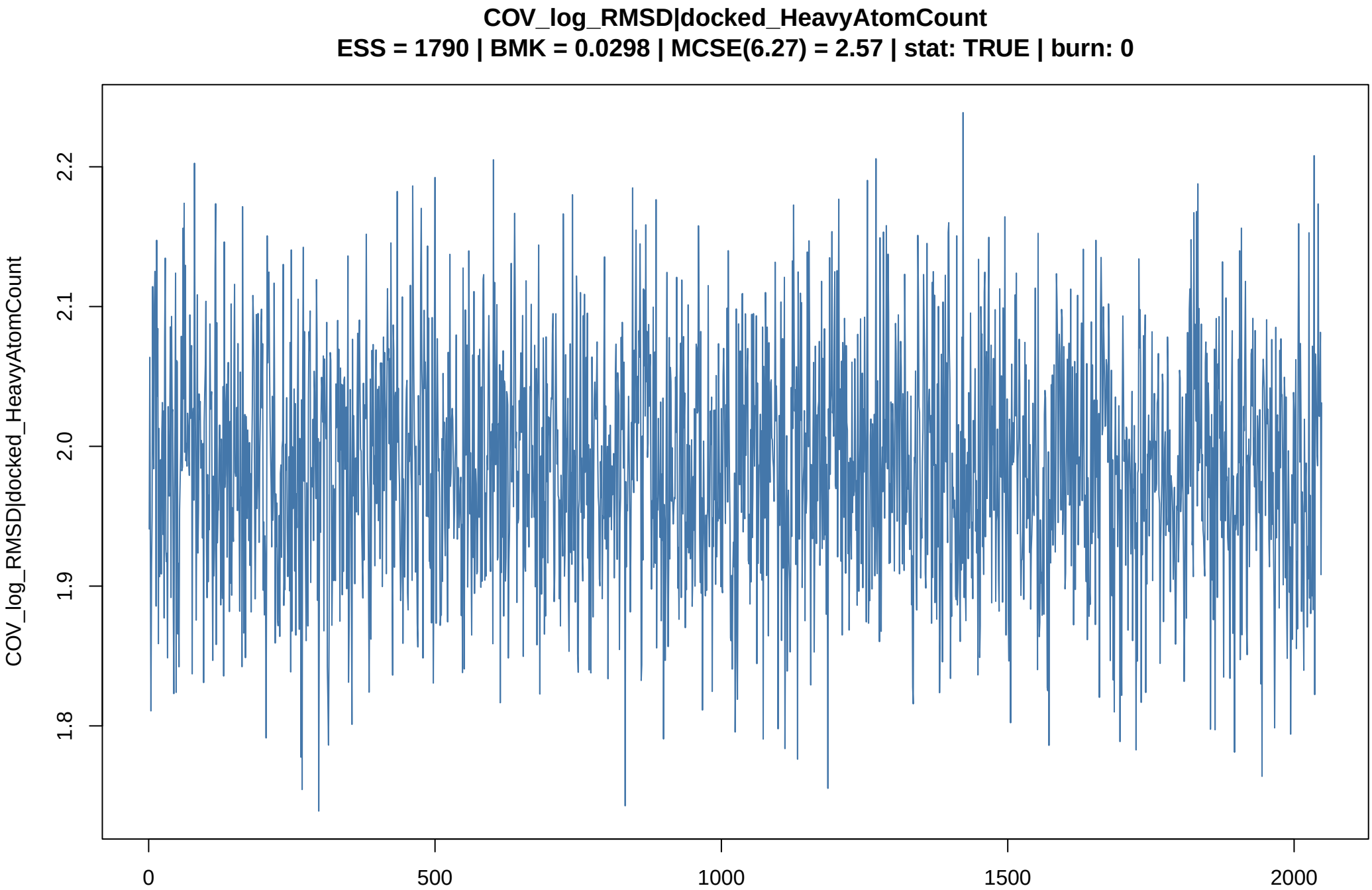

VAR_template_HeavyAtomCount
ESS = 1810 | BMK = 0.0508 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
4.22
0
500
1000
1500
2000

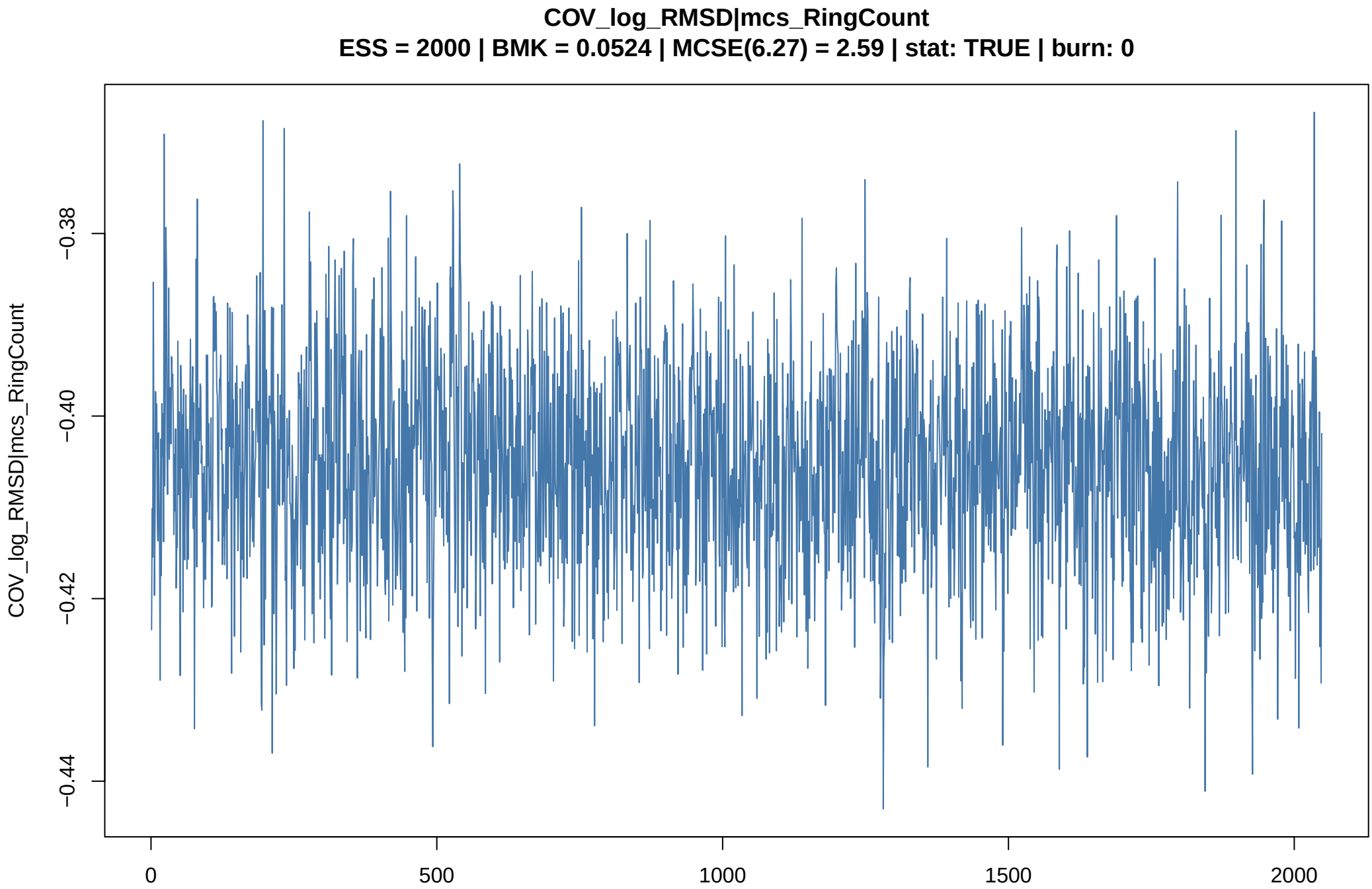

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0476 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
0.85
0.90
0.95
0
500
1000
1500
2000

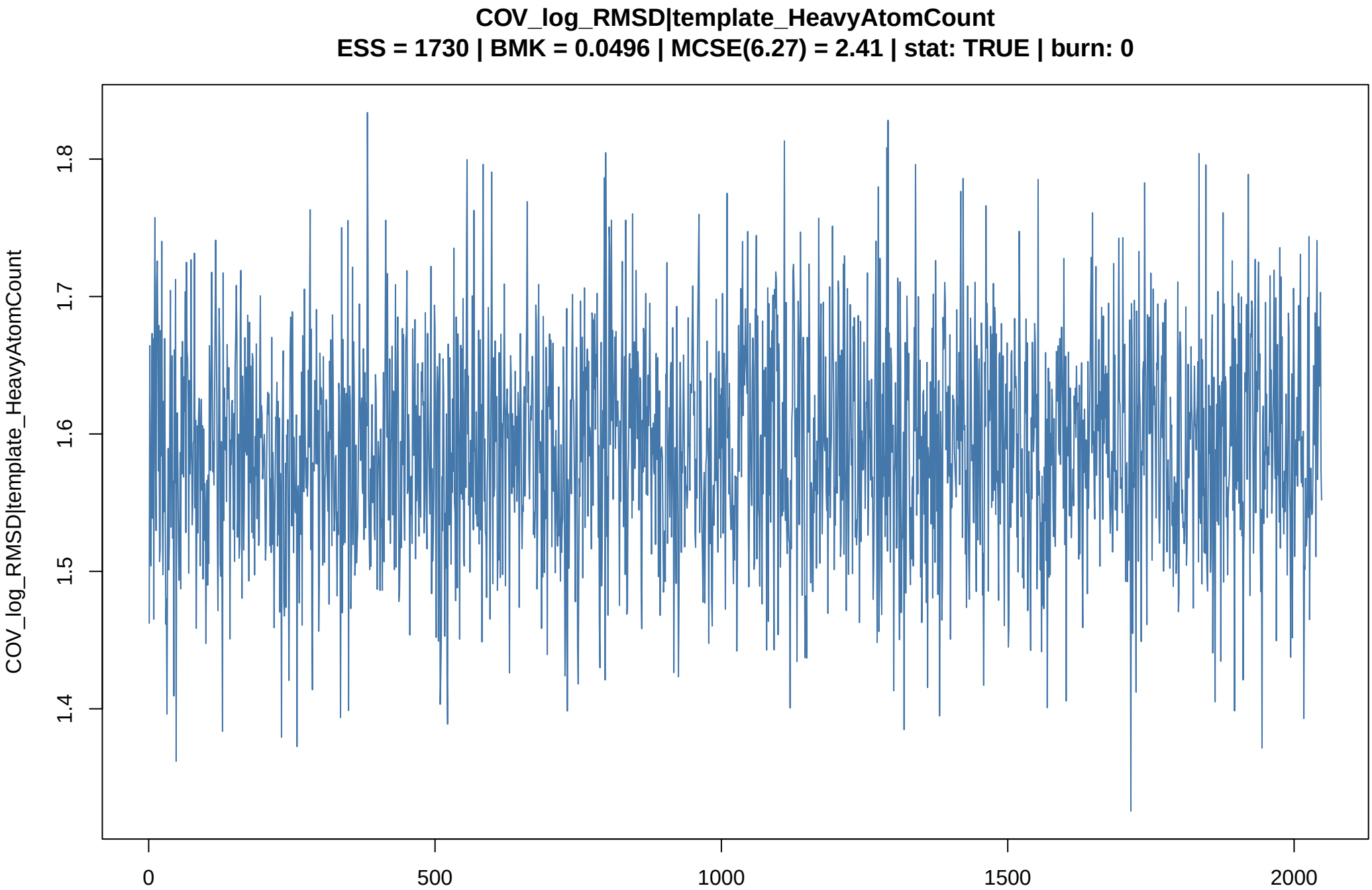

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0531 | MCSE(6.27) = 1.81 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

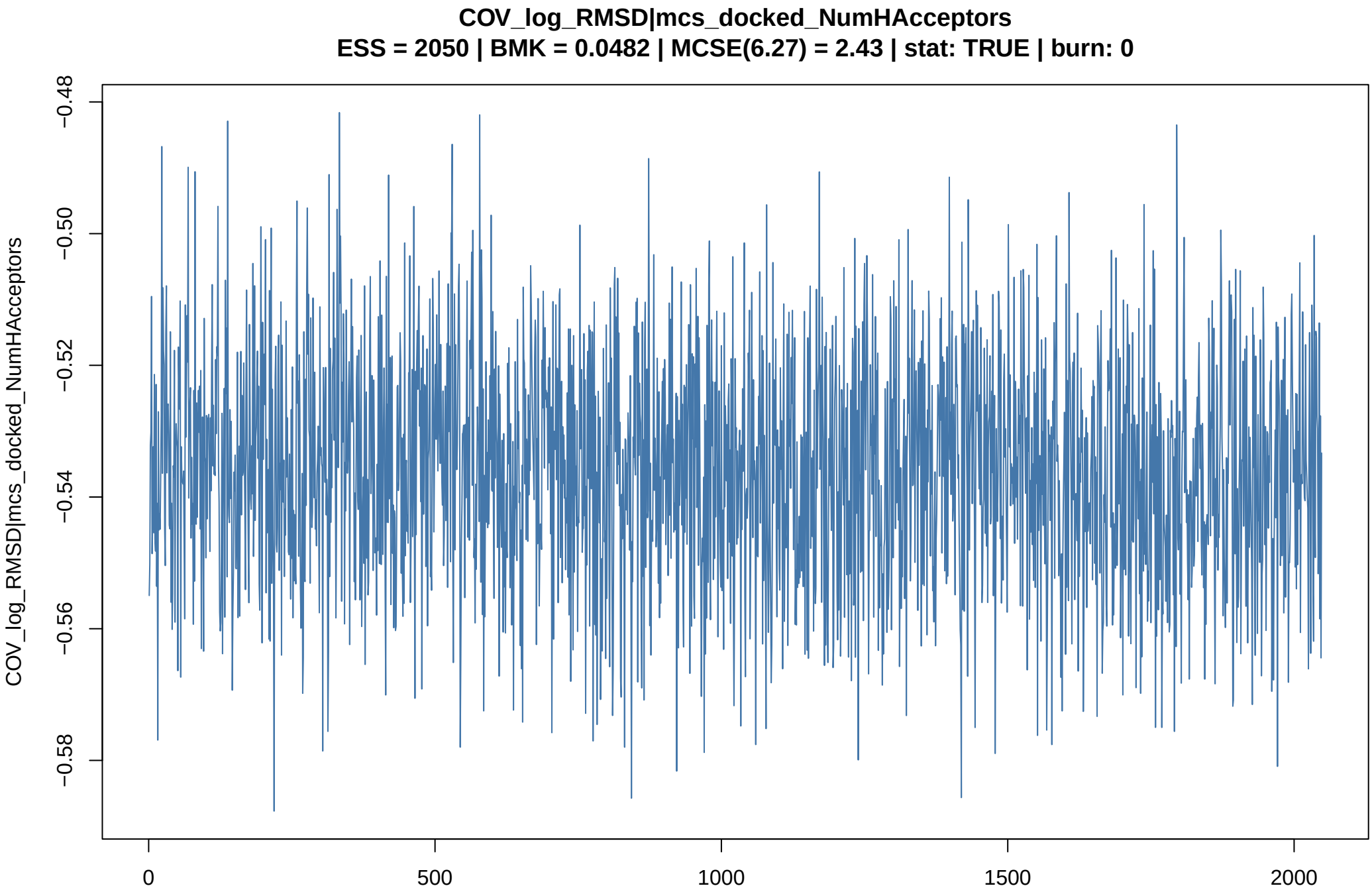

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0448 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
1.44
1.46
1.48
1.50
1.52
1.54
1.56
0
500
1000
1500
2000

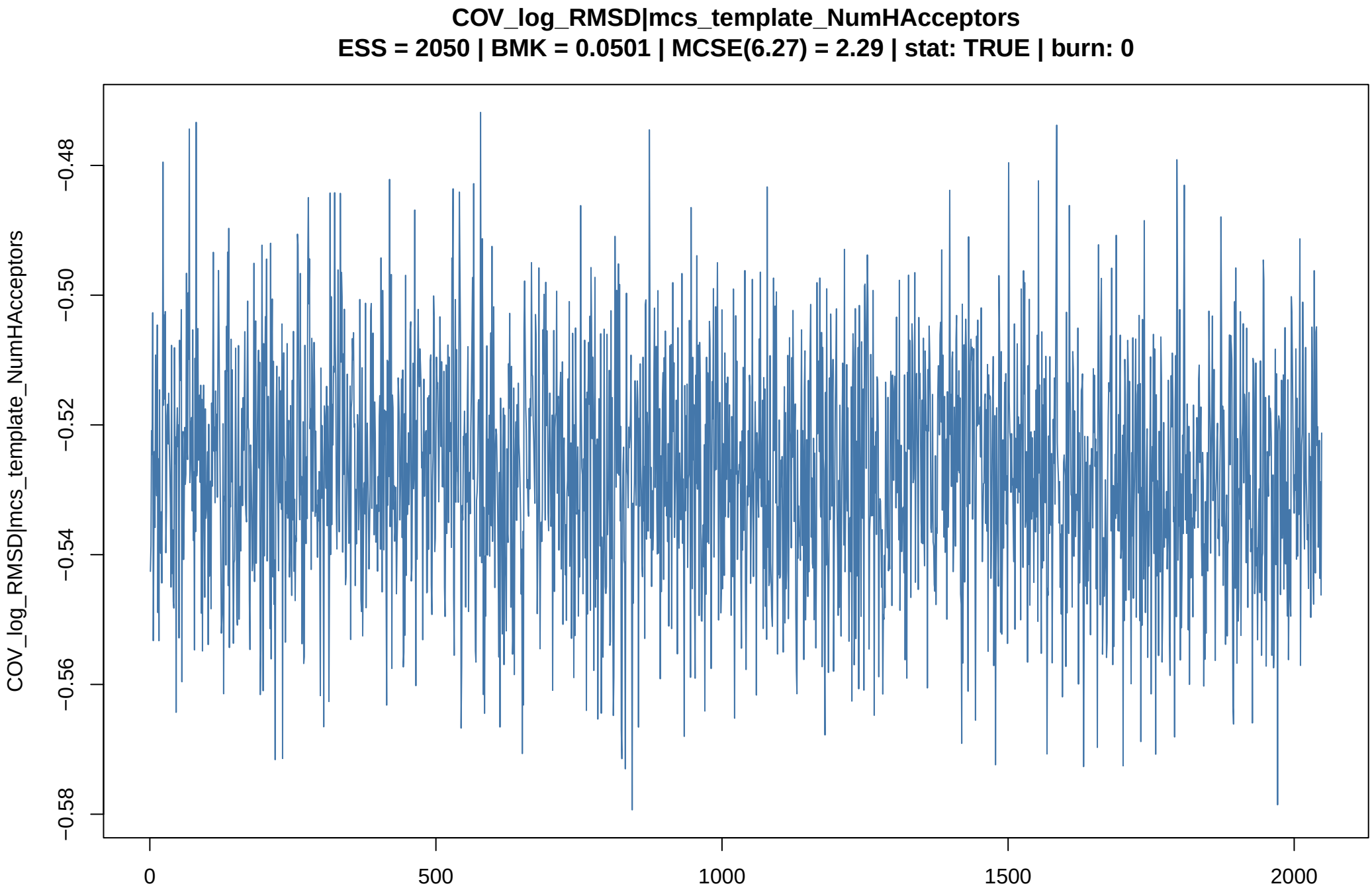

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1710 | BMK = 0.0386 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

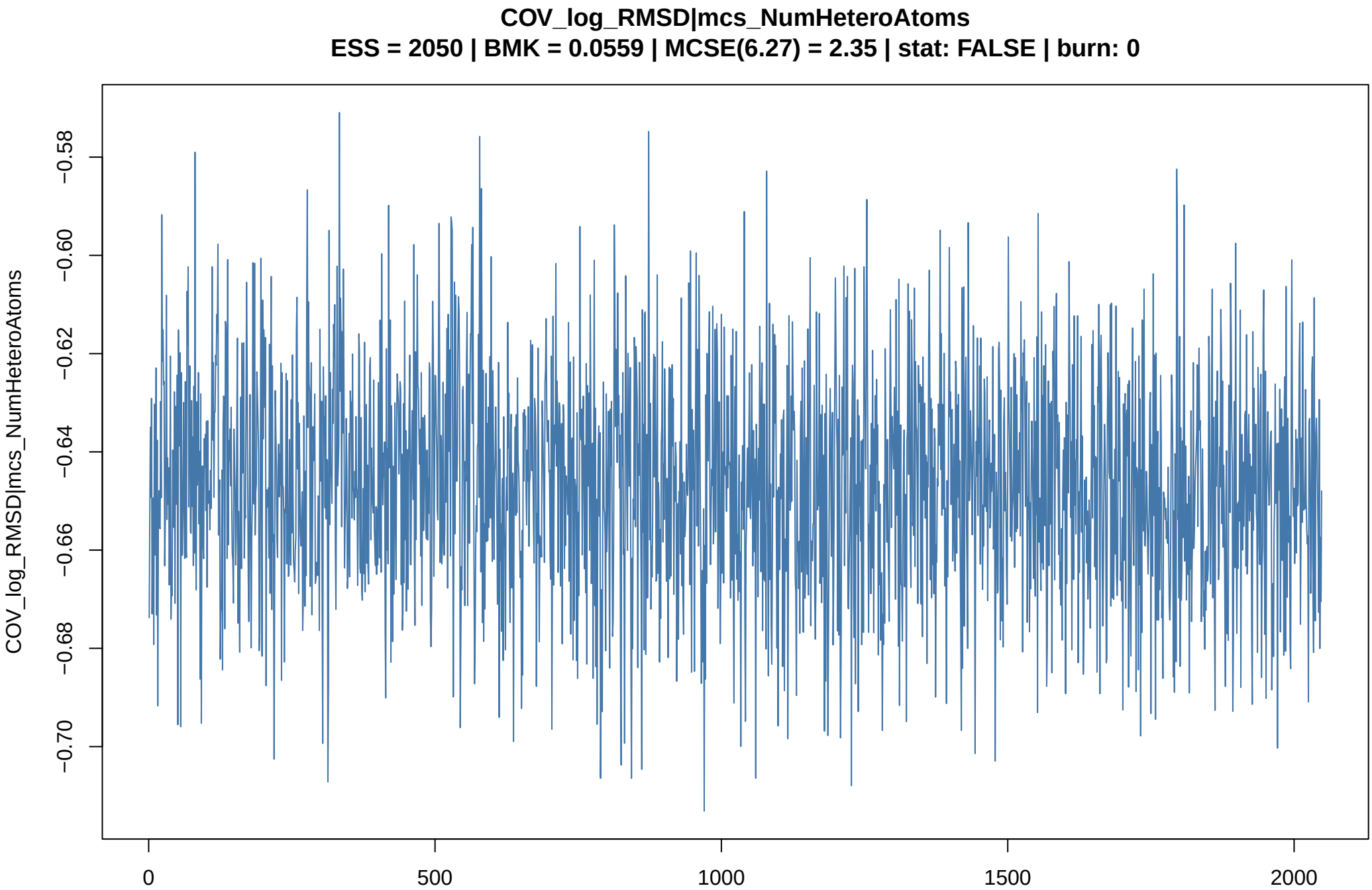

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1790 | BMK = 0.0298 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

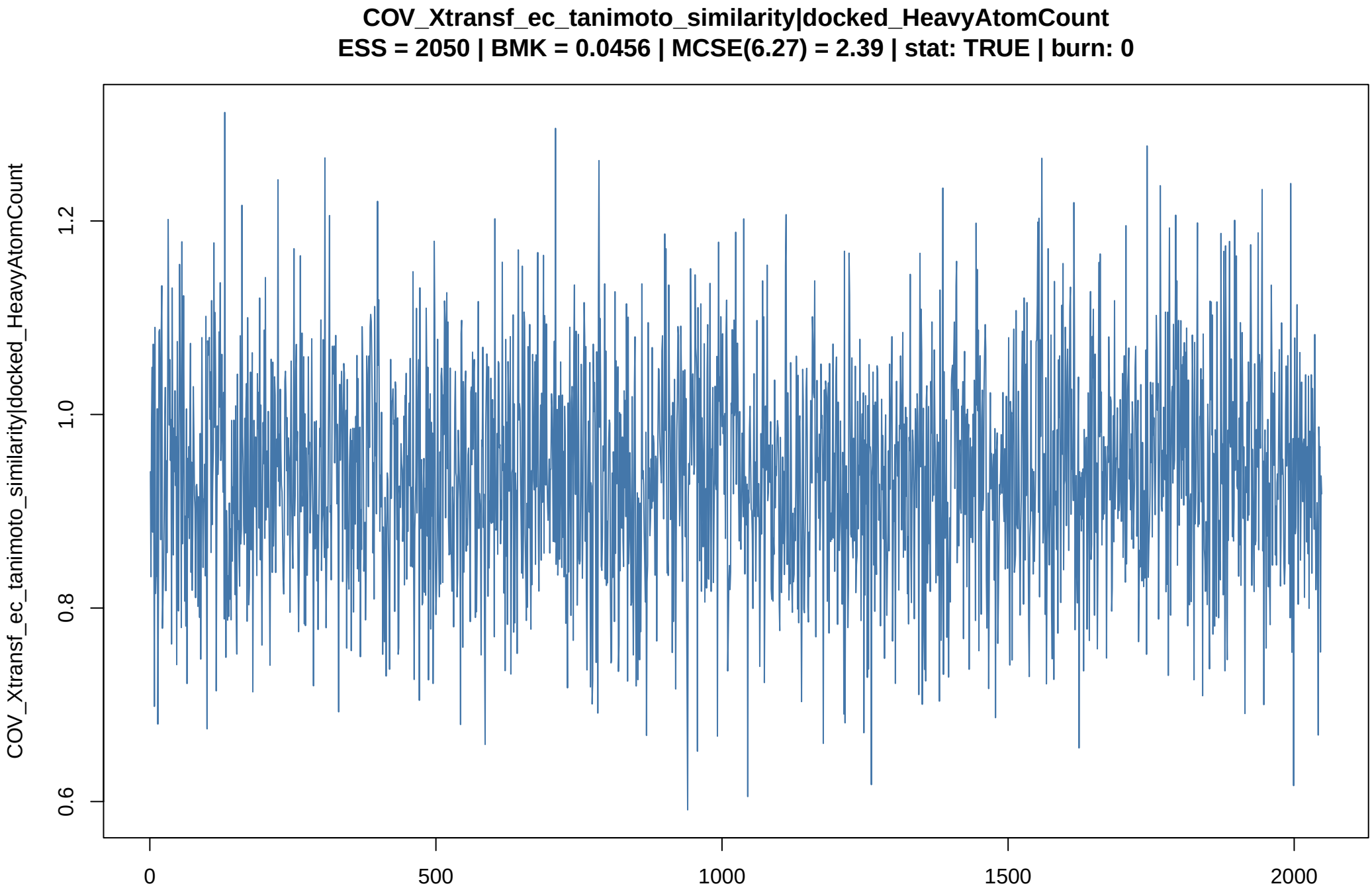

COV_log_RMSD|mcs_RingCount
ESS = 2000 | BMK = 0.0524 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.38
−0.40
−0.42
−0.44
0
500
1000
1500
2000

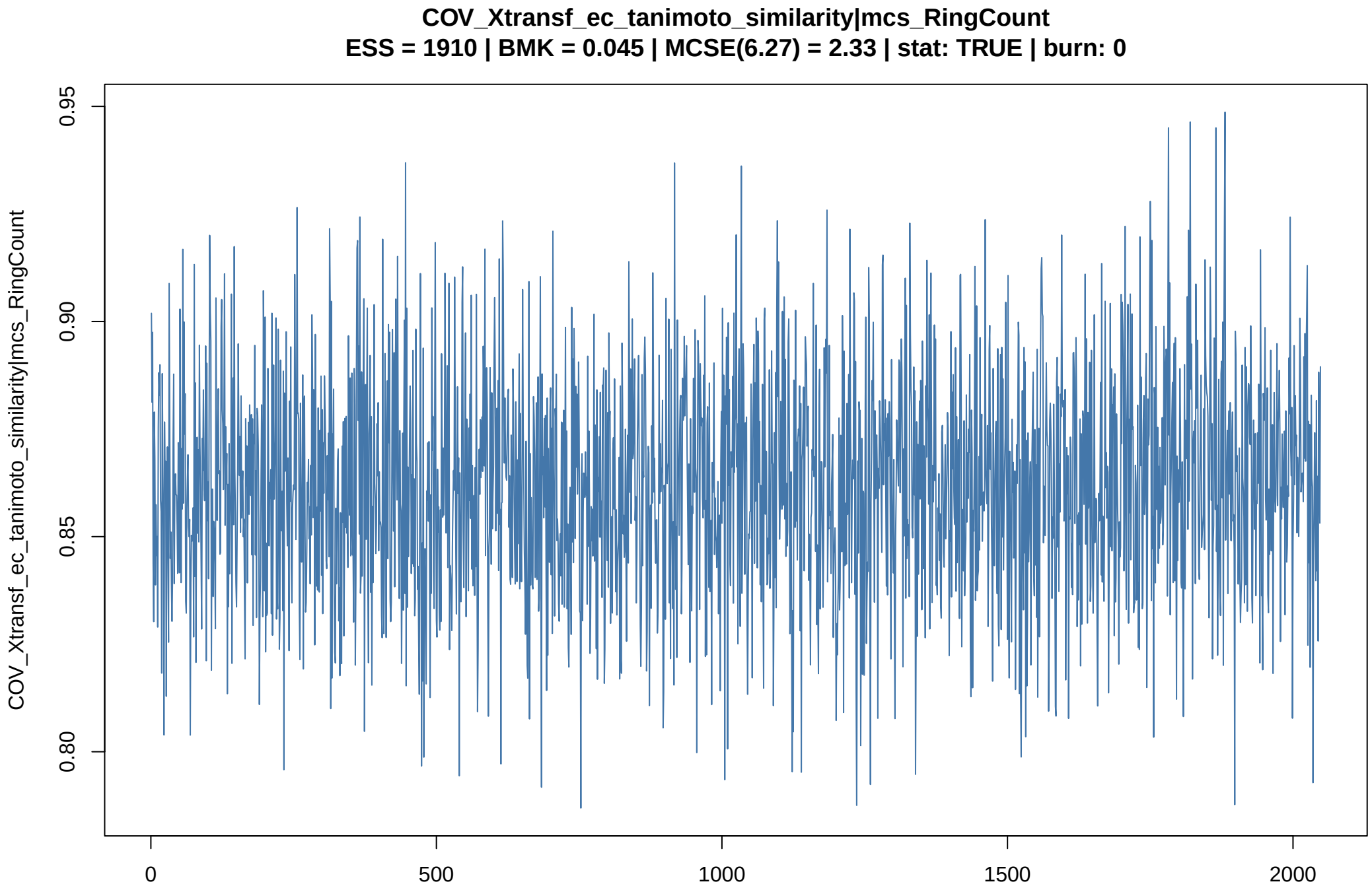

COV_log_RMSD|template_HeavyAtomCount
ESS = 1730 | BMK = 0.0496 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

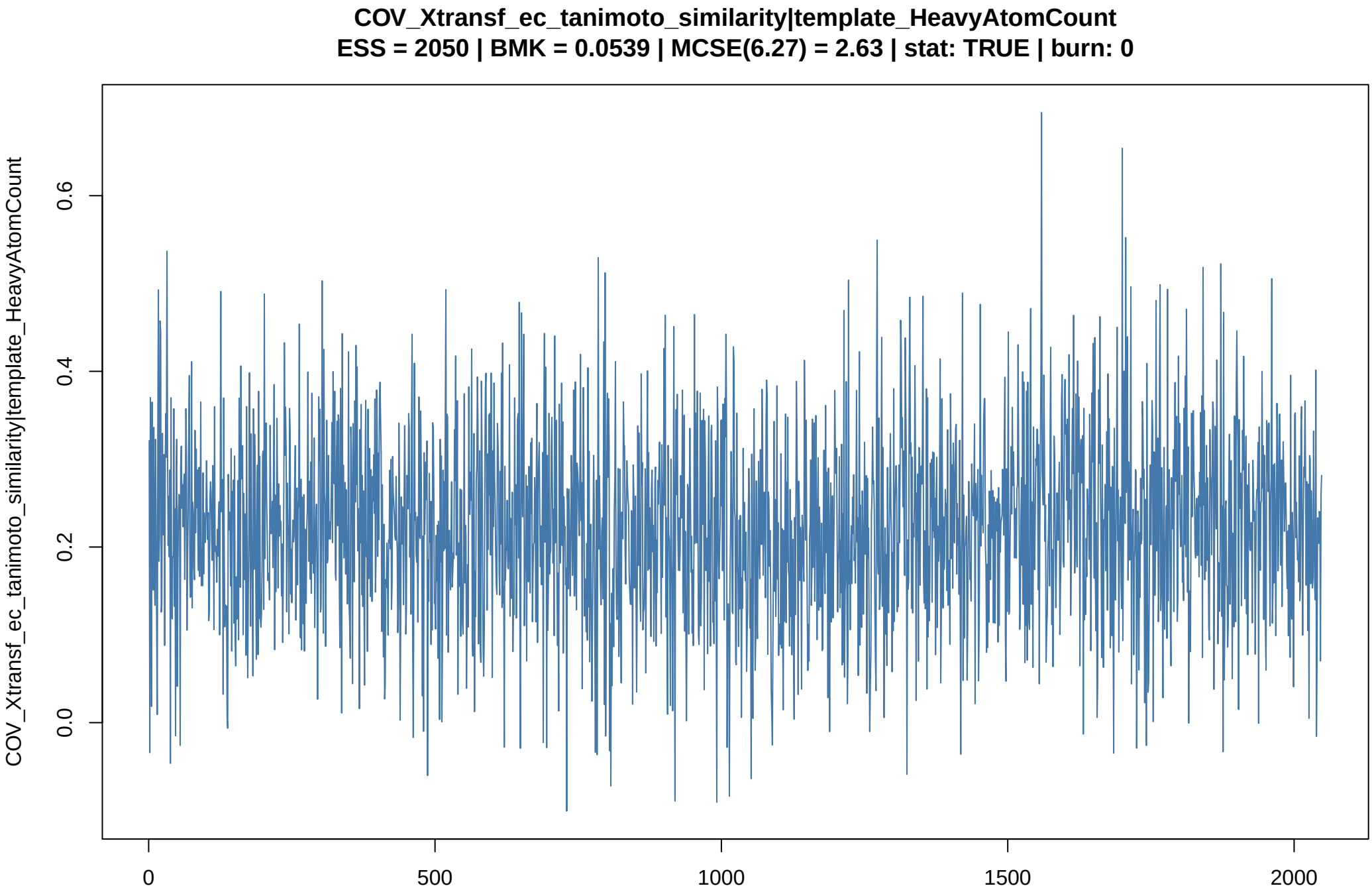

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

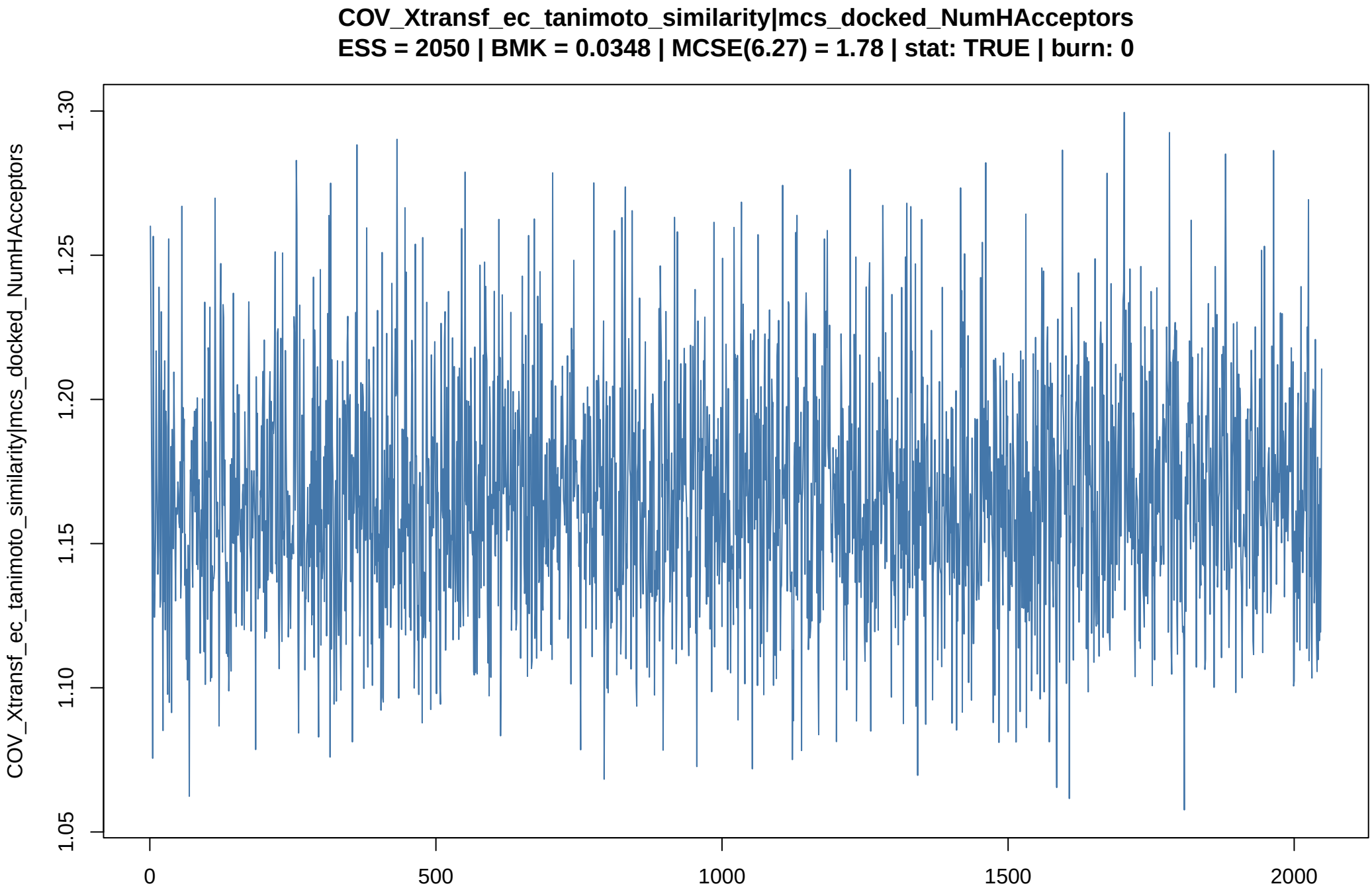

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0501 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

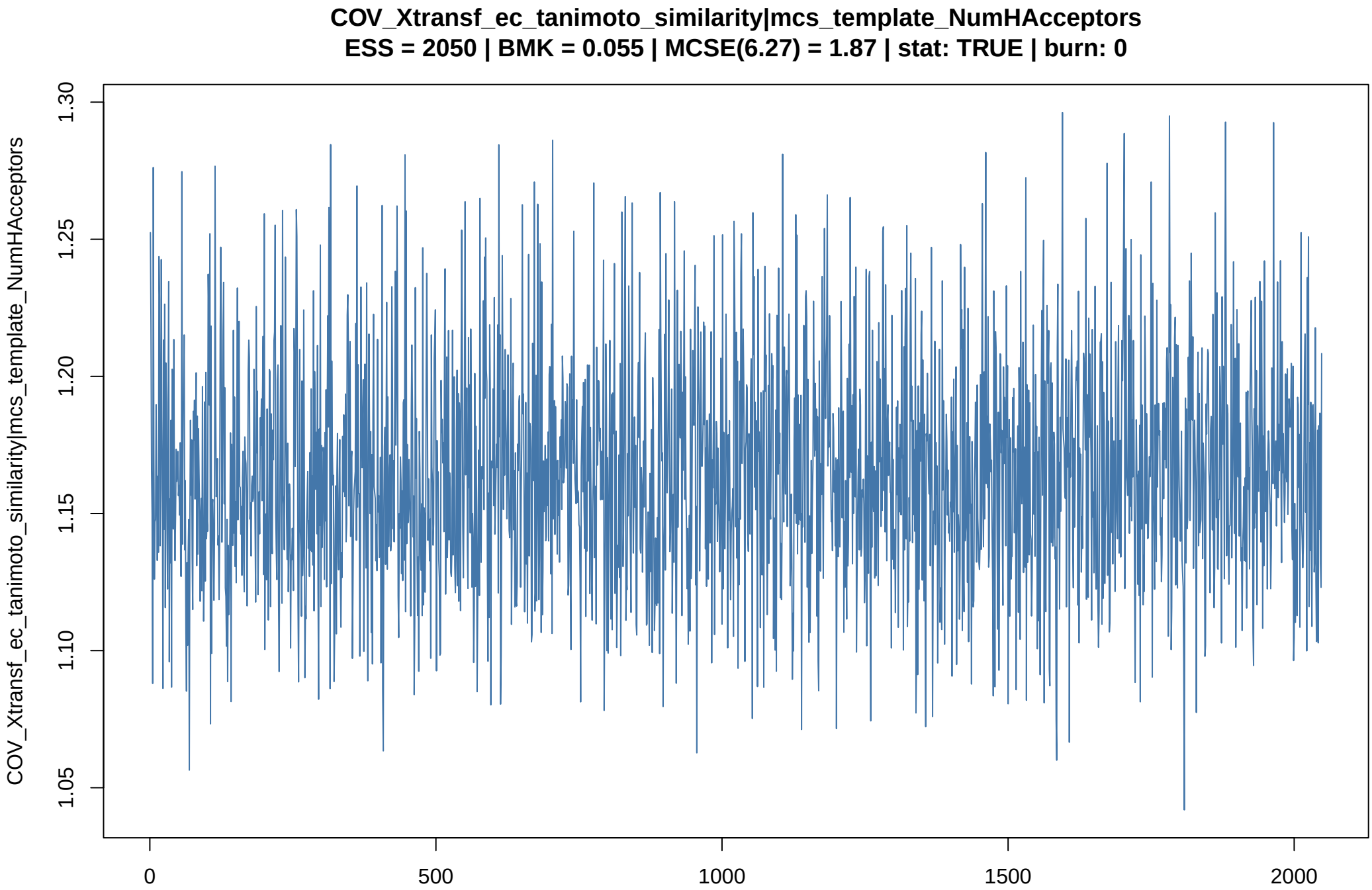

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0559 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.58
−0.60
−0.62
−0.64
−0.66
−0.68
−0.70
0
500
1000
1500
2000

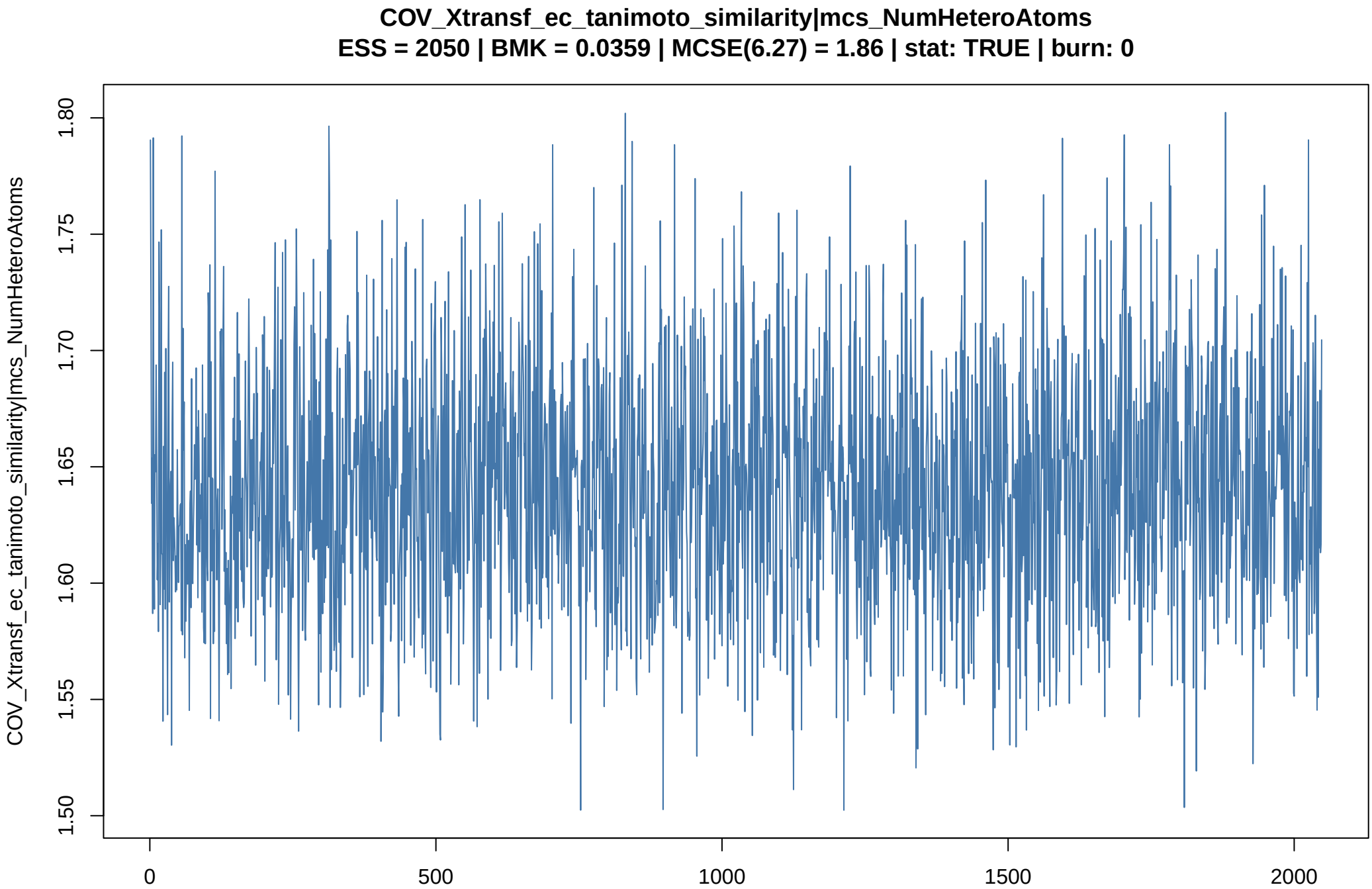

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0456 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

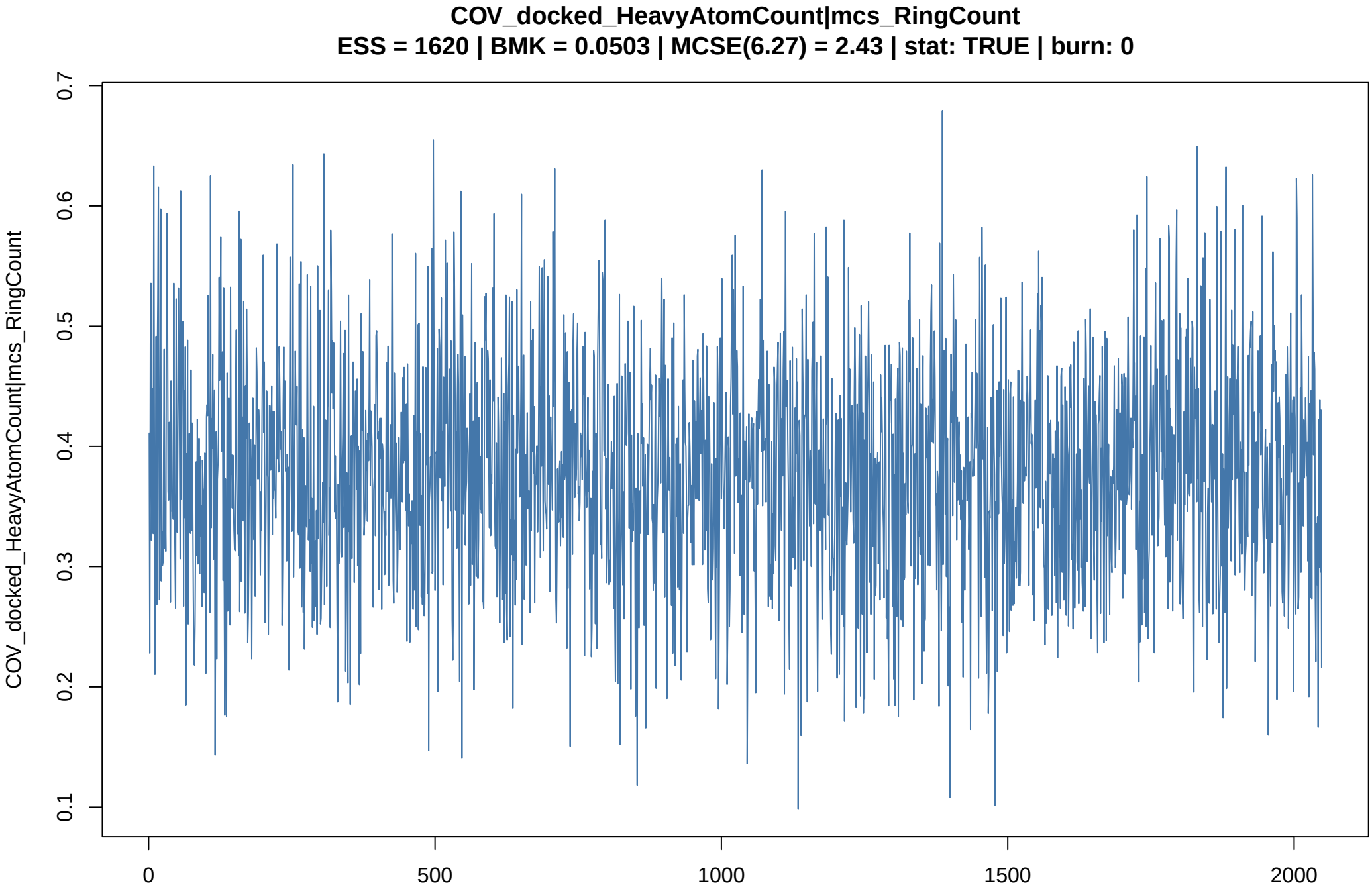

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1910 | BMK = 0.045 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

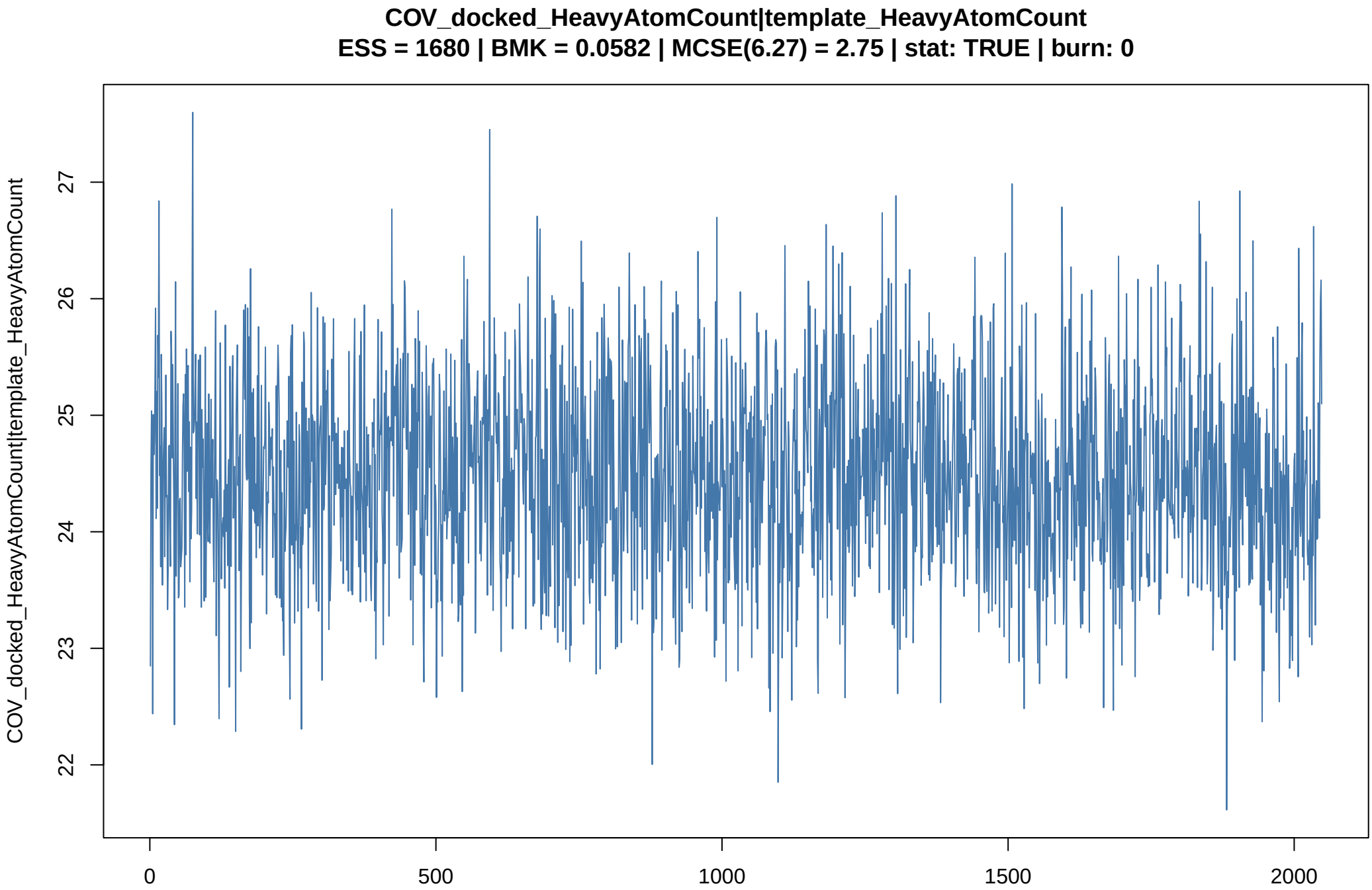

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 2050 | BMK = 0.0539 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.0
0.2
0.4
0.6
0
500
1000
1500
2000

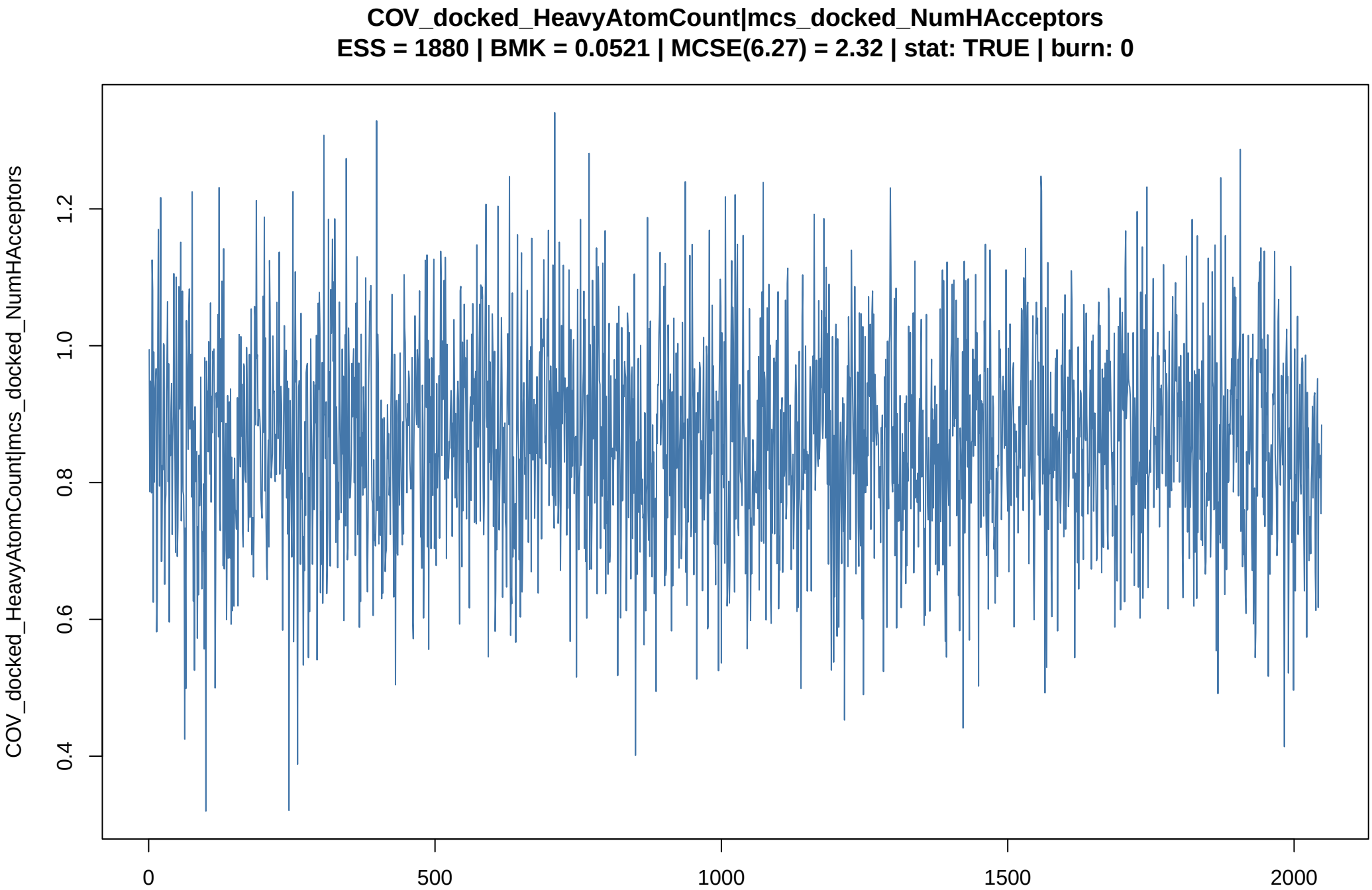

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0348 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

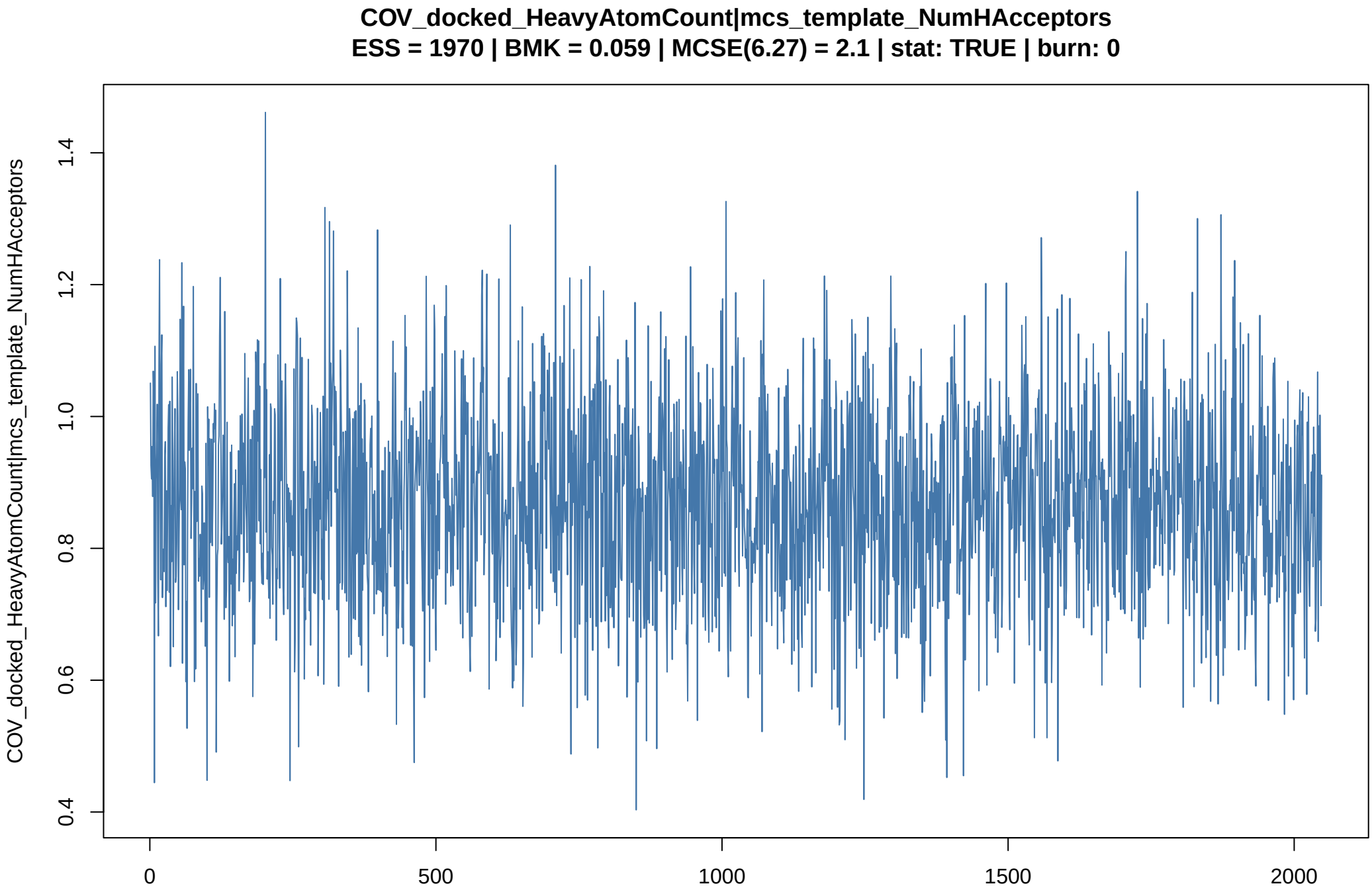

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.055 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.30
1.25
1.20
1.15
1.10
1.05
0
500
1000
1500
2000

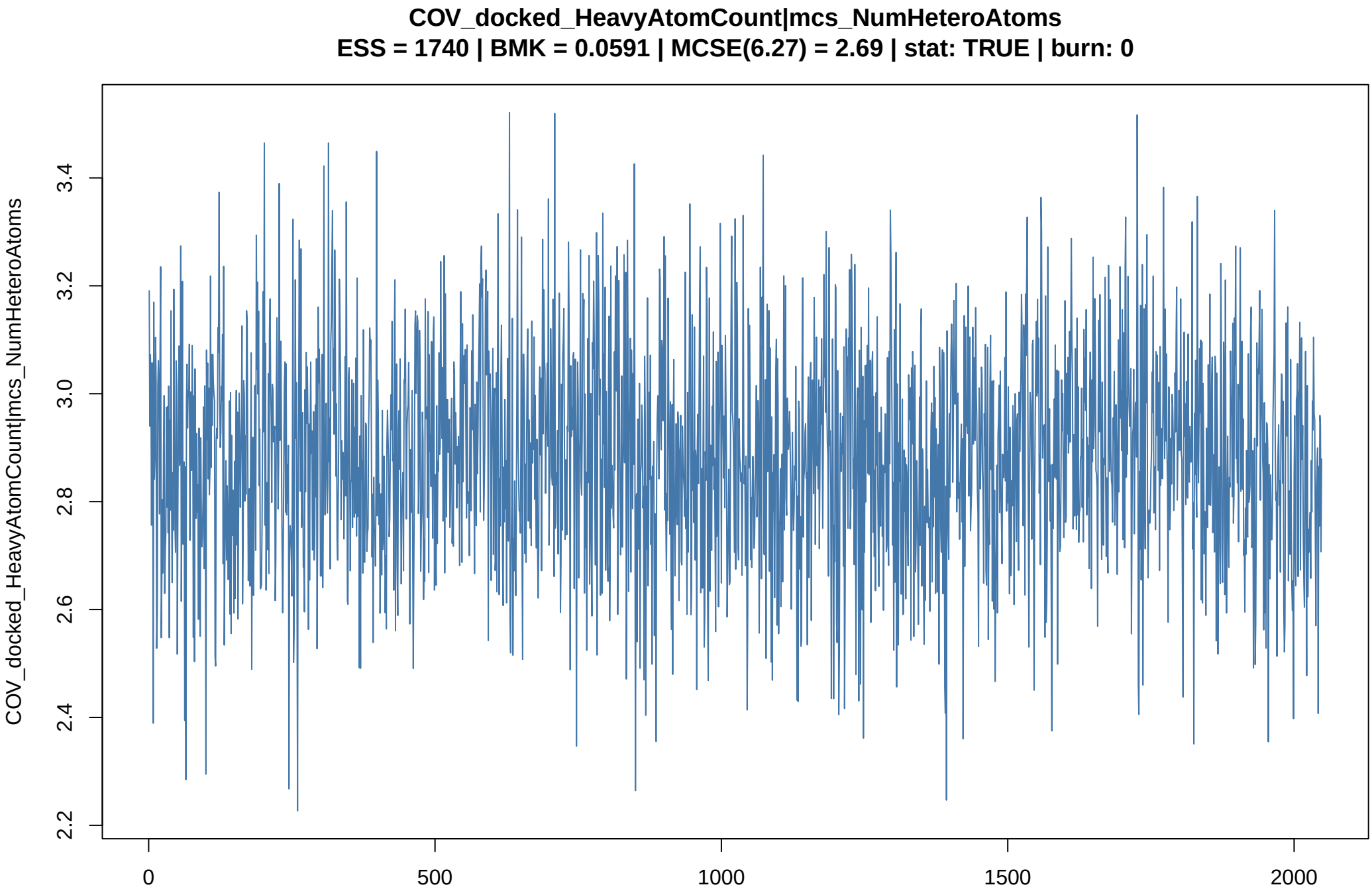

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0359 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.50
1.55
1.60
1.65
1.70
1.75
1.80
0
500
1000
1500
2000

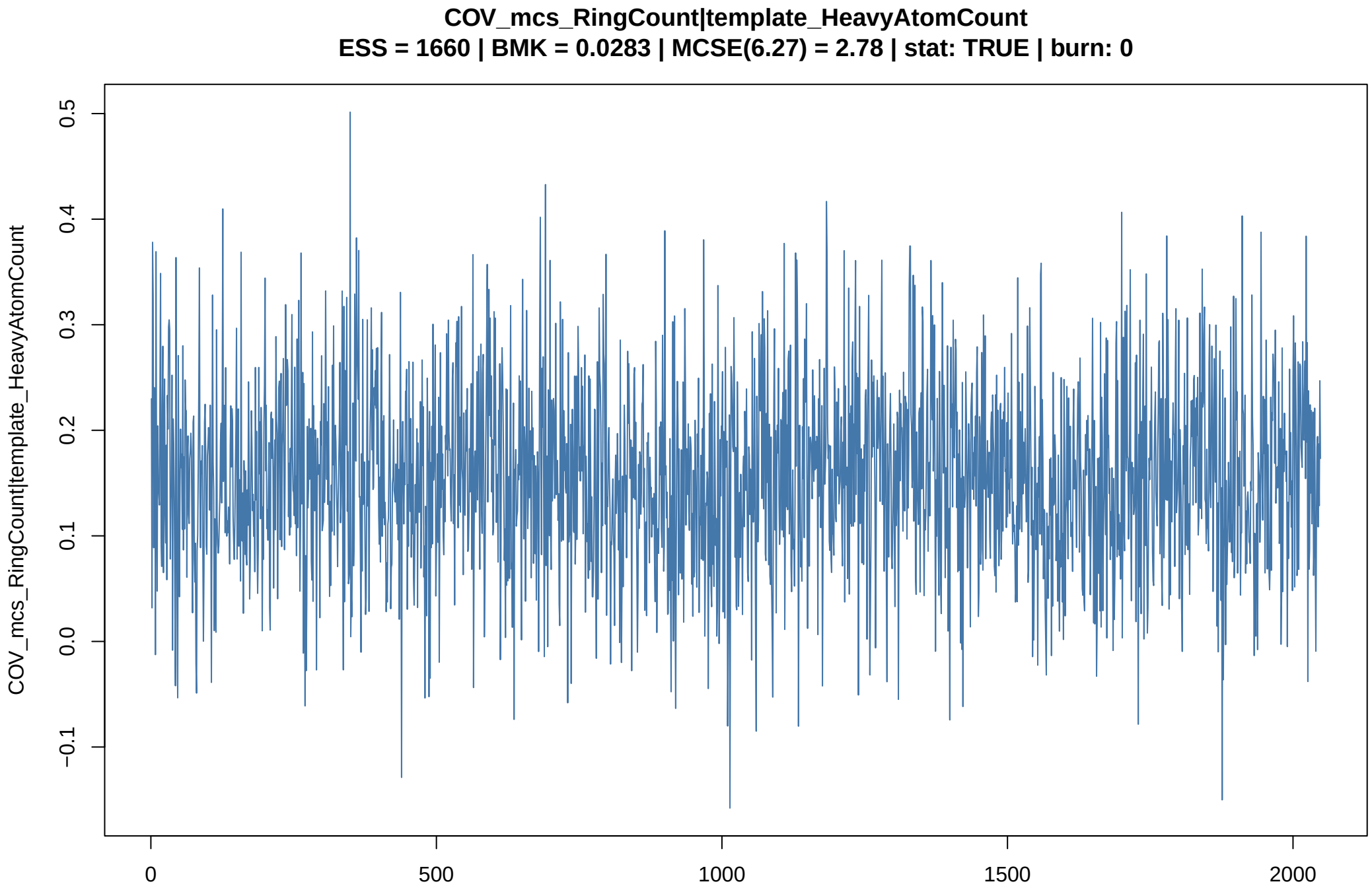

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1620 | BMK = 0.0503 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

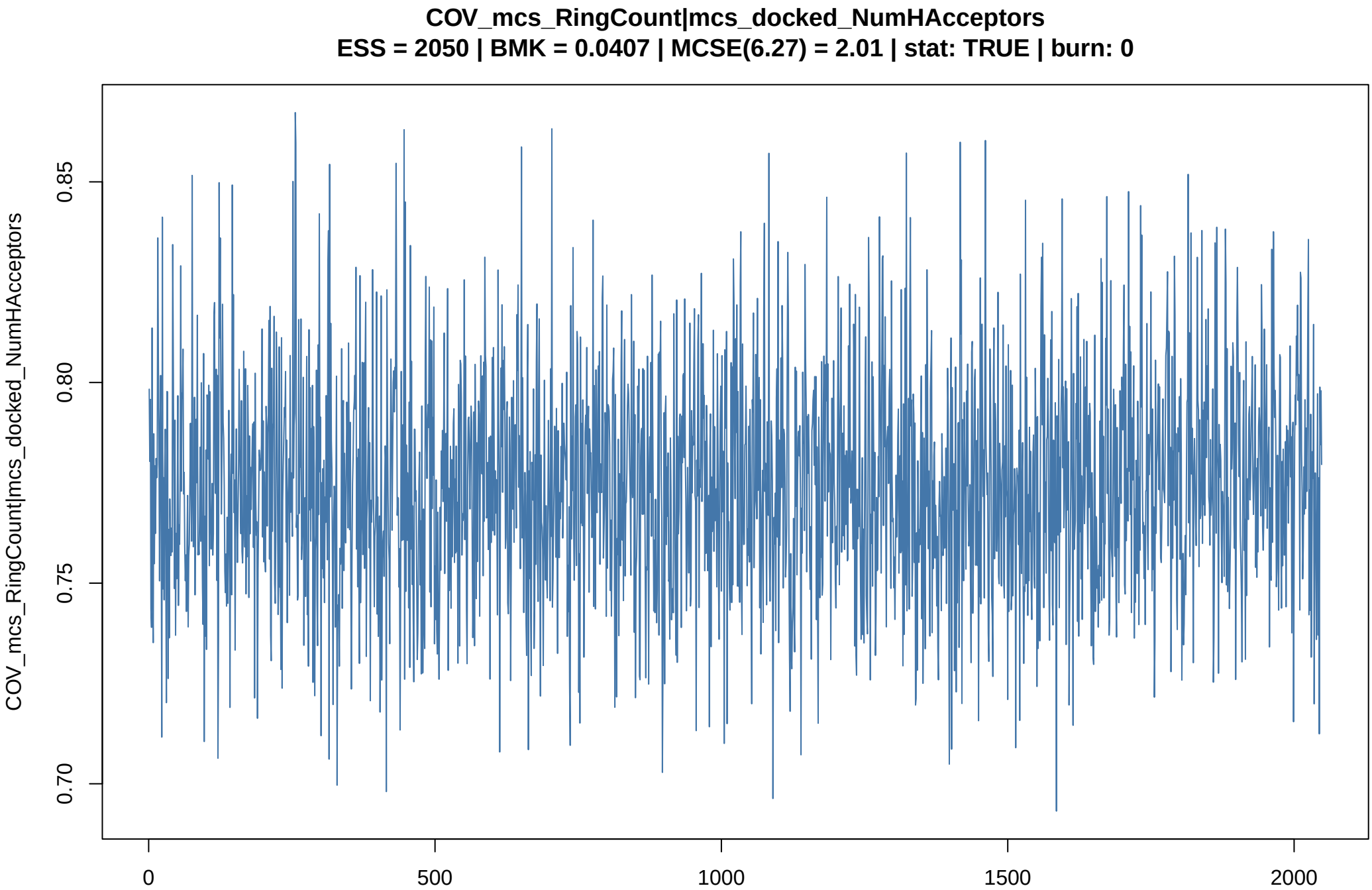

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1680 | BMK = 0.0582 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
0
500
1000
1500
2000

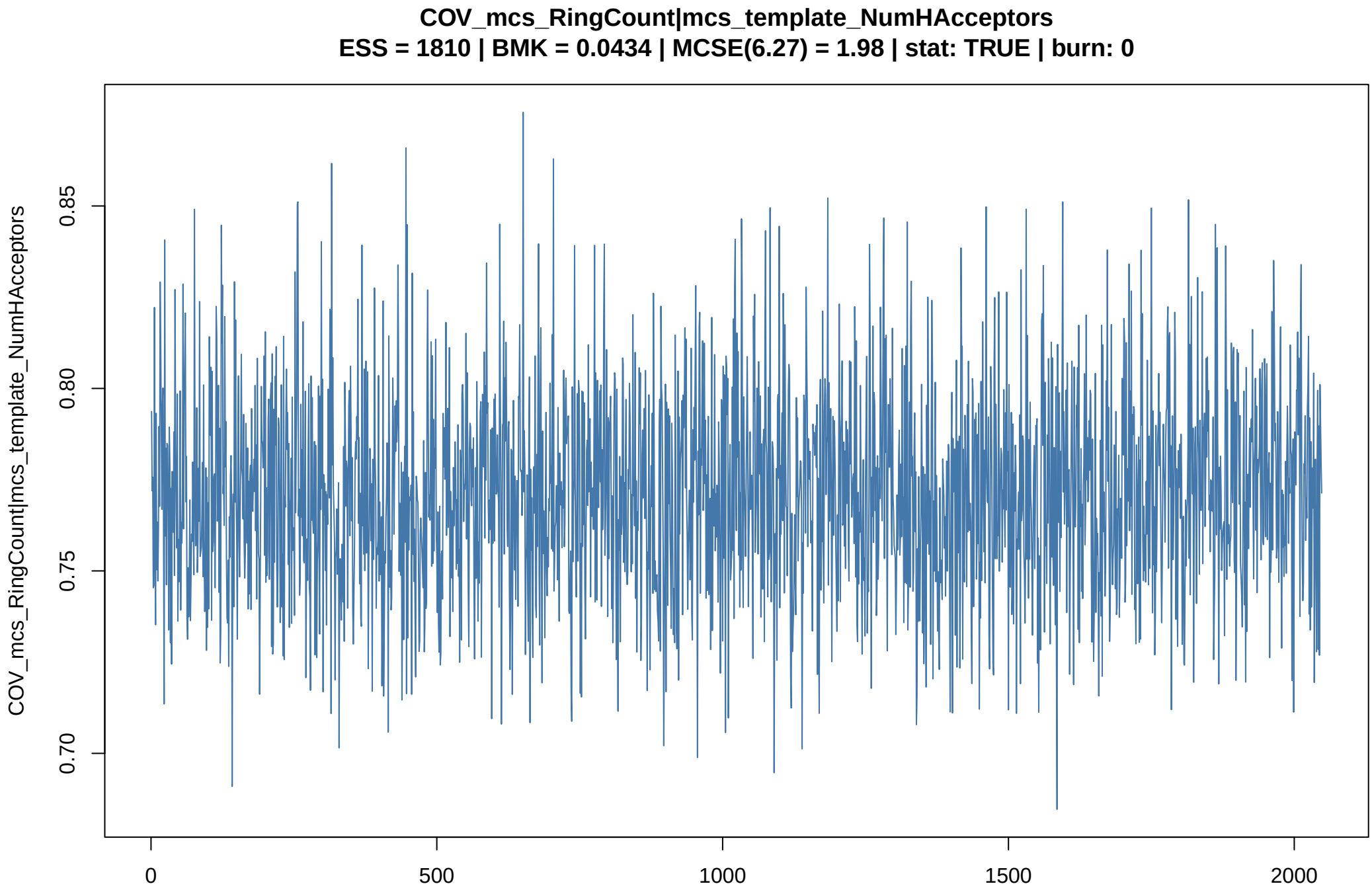

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1880 | BMK = 0.0521 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

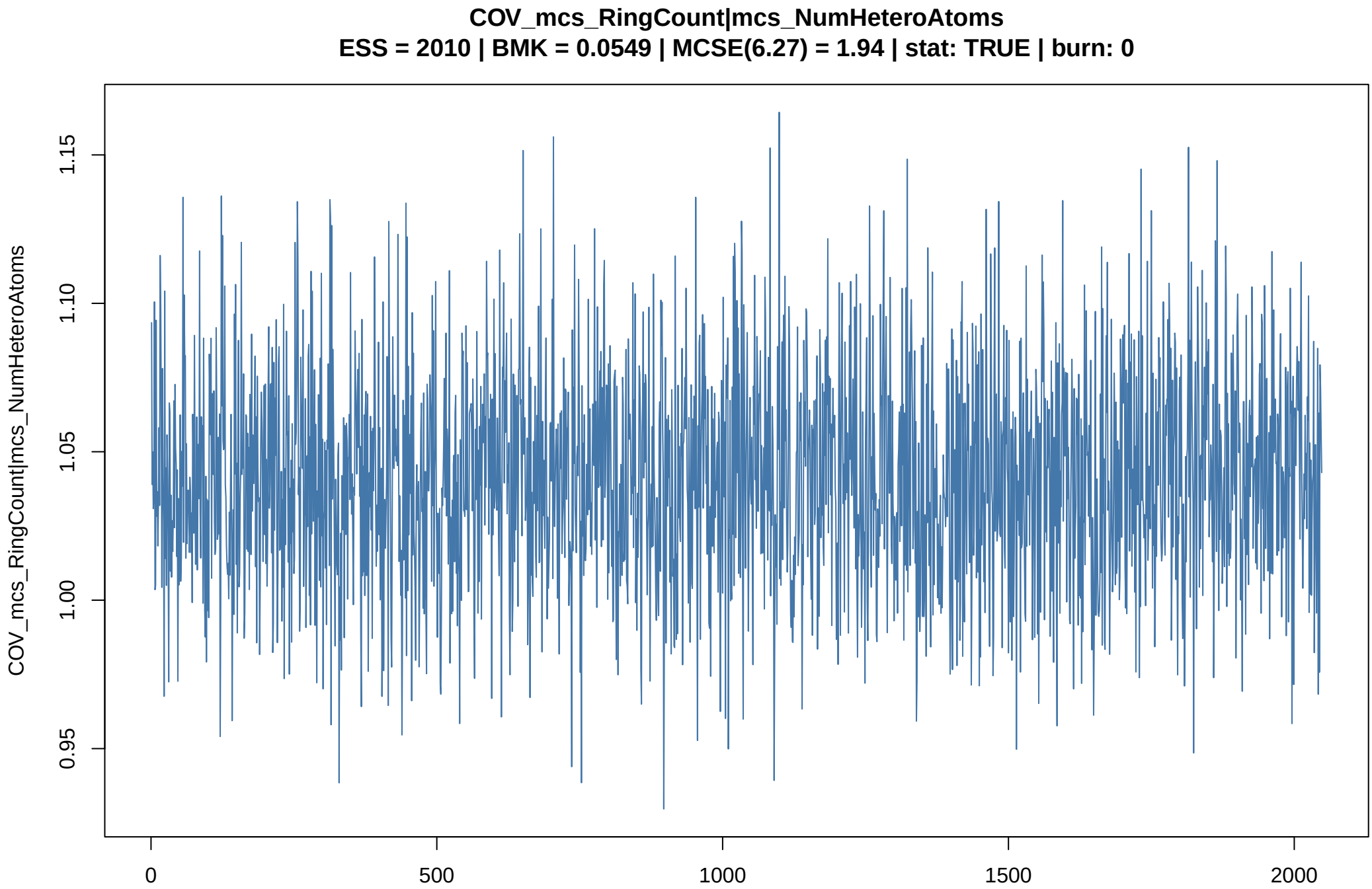

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1970 | BMK = 0.059 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

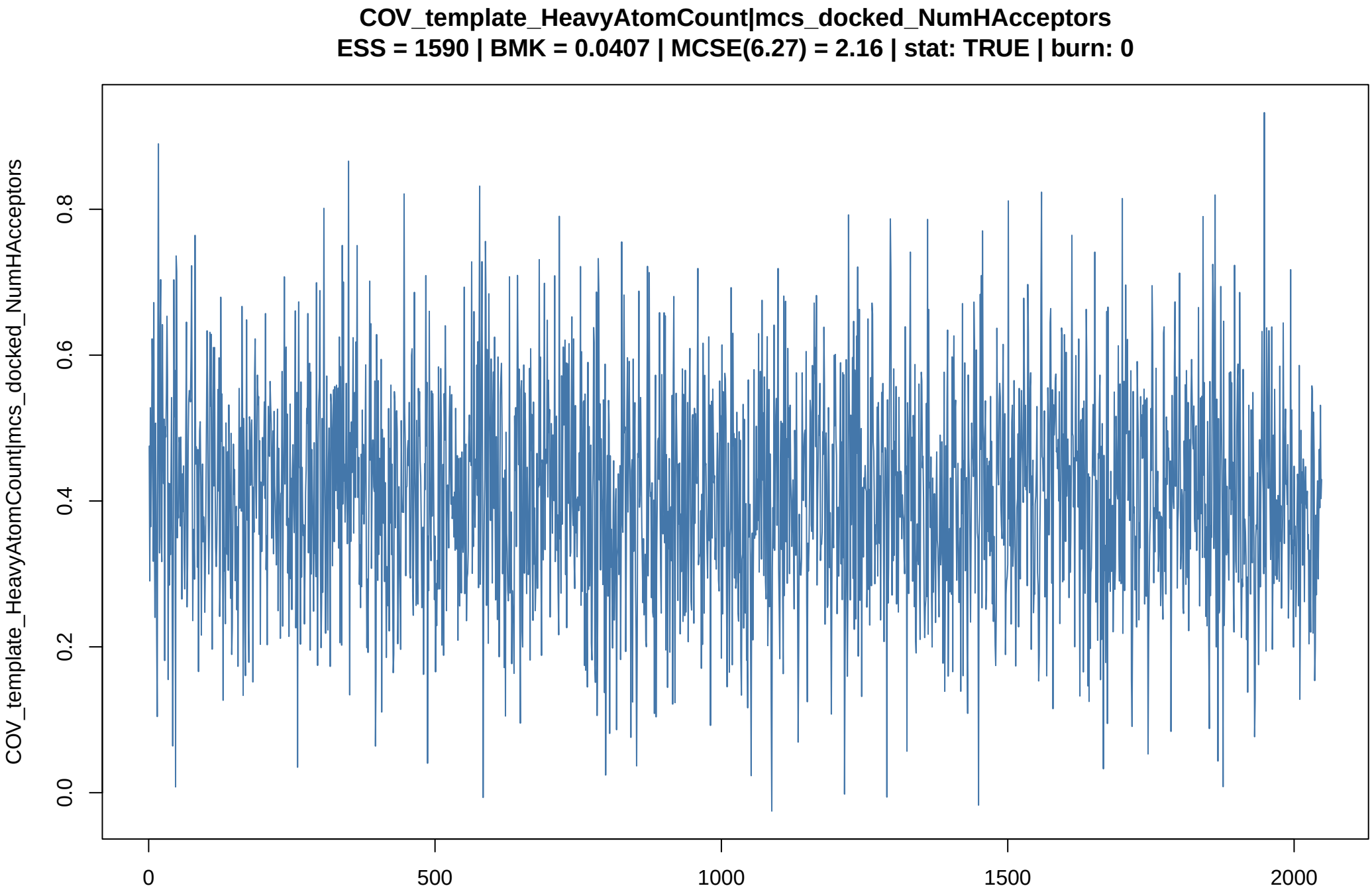

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1740 | BMK = 0.0591 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
3.2
3.4
0
500
1000
1500
2000

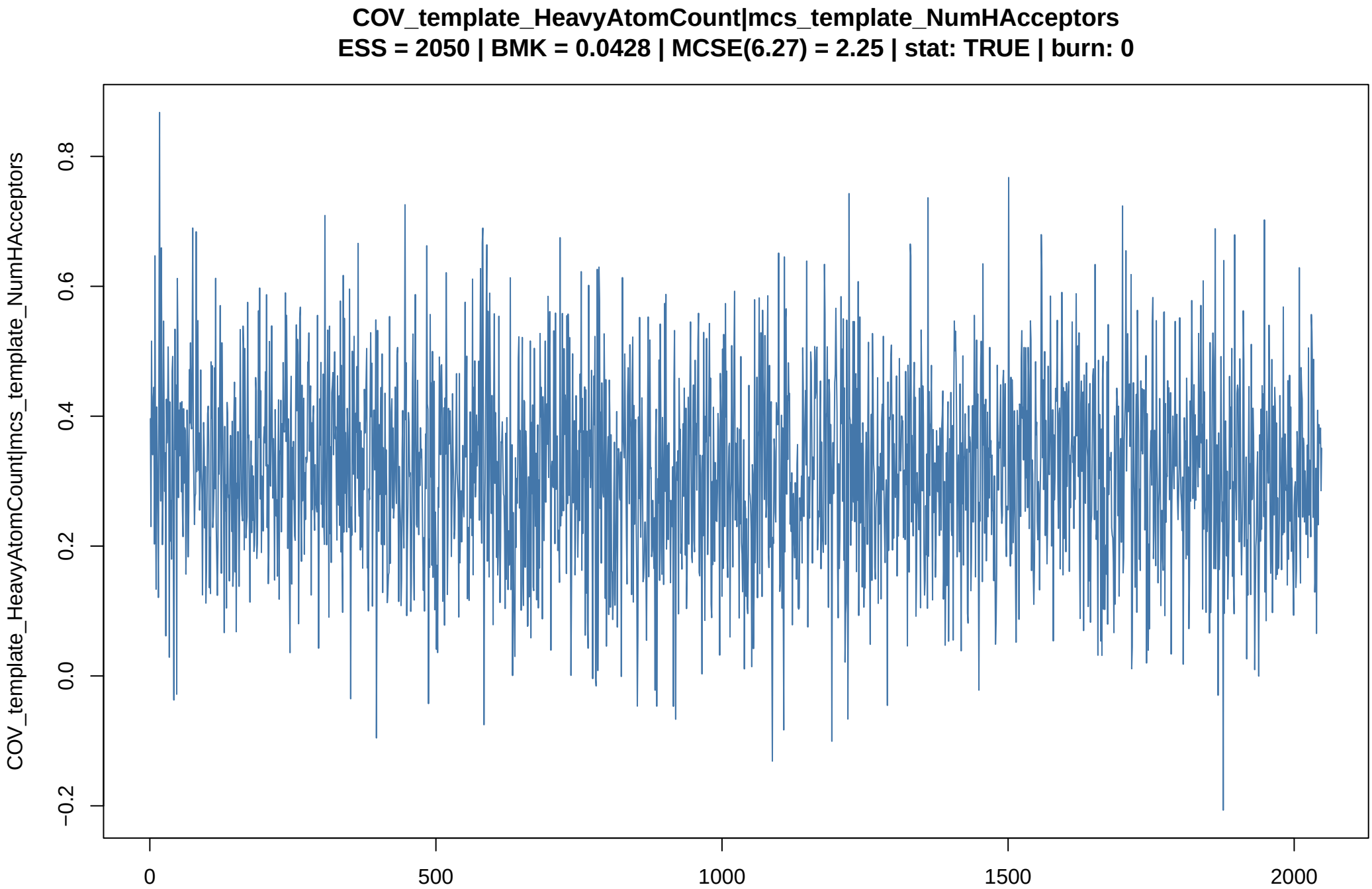

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1660 | BMK = 0.0283 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

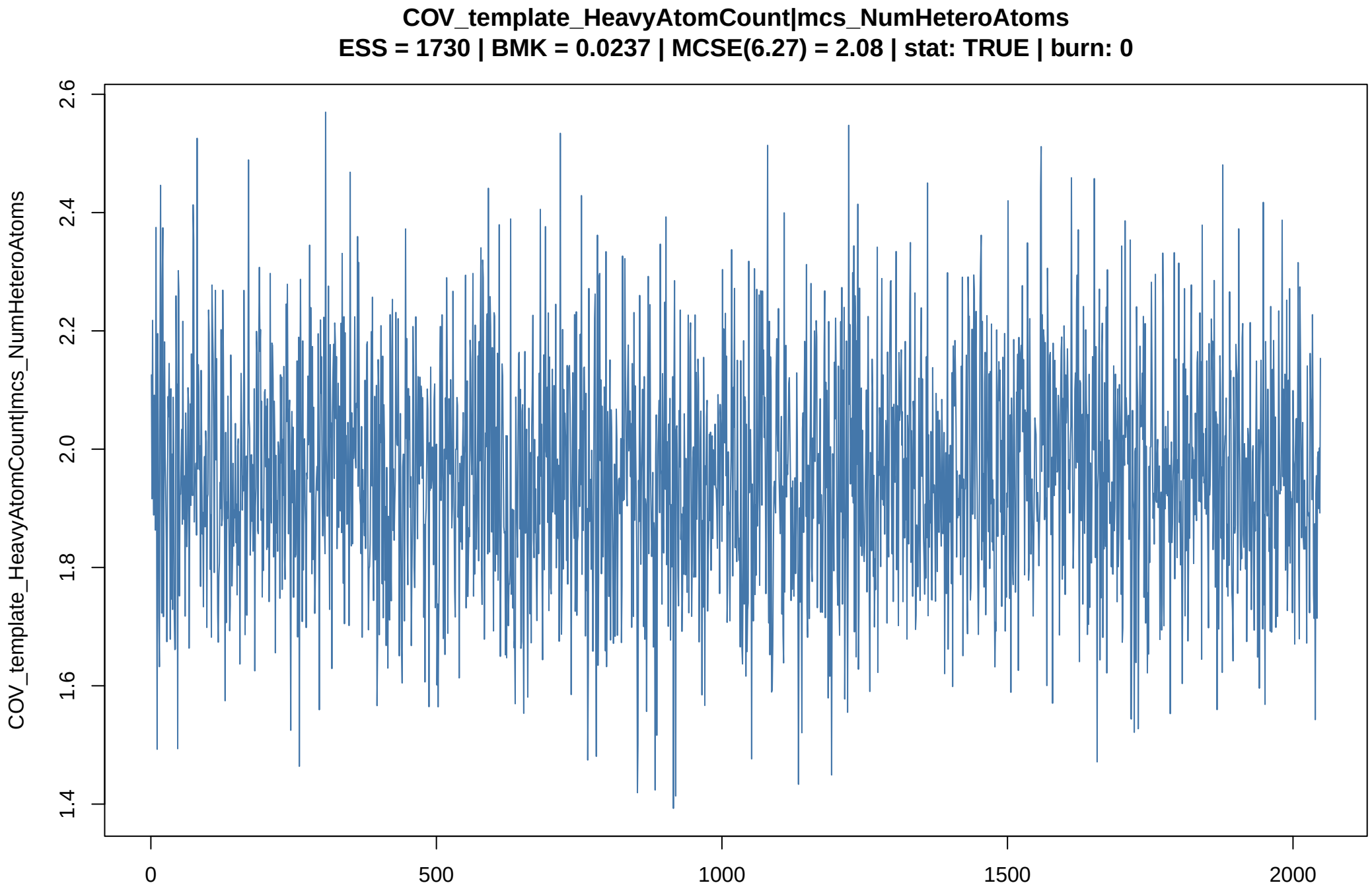

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

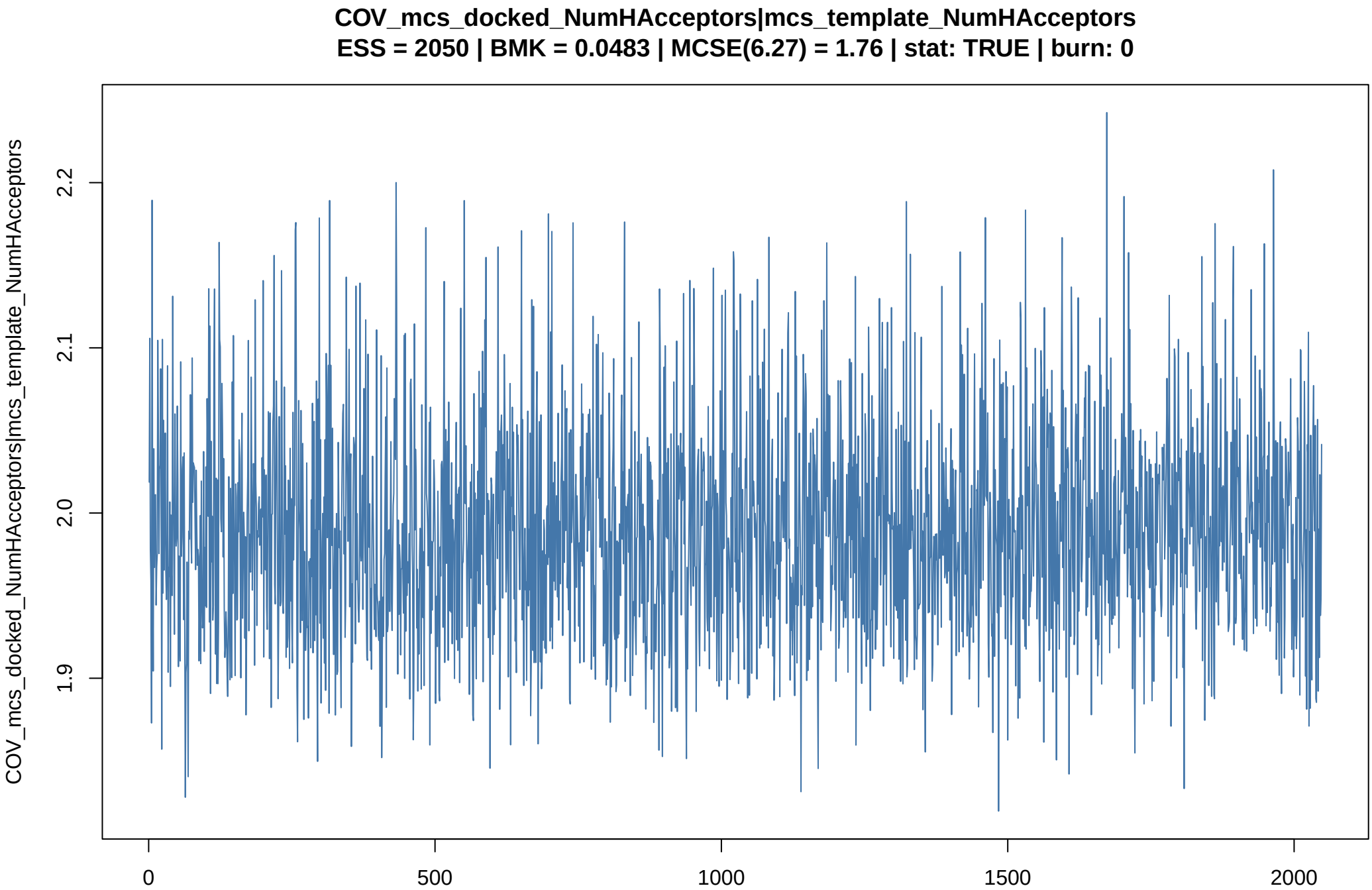

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 1810 | BMK = 0.0434 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

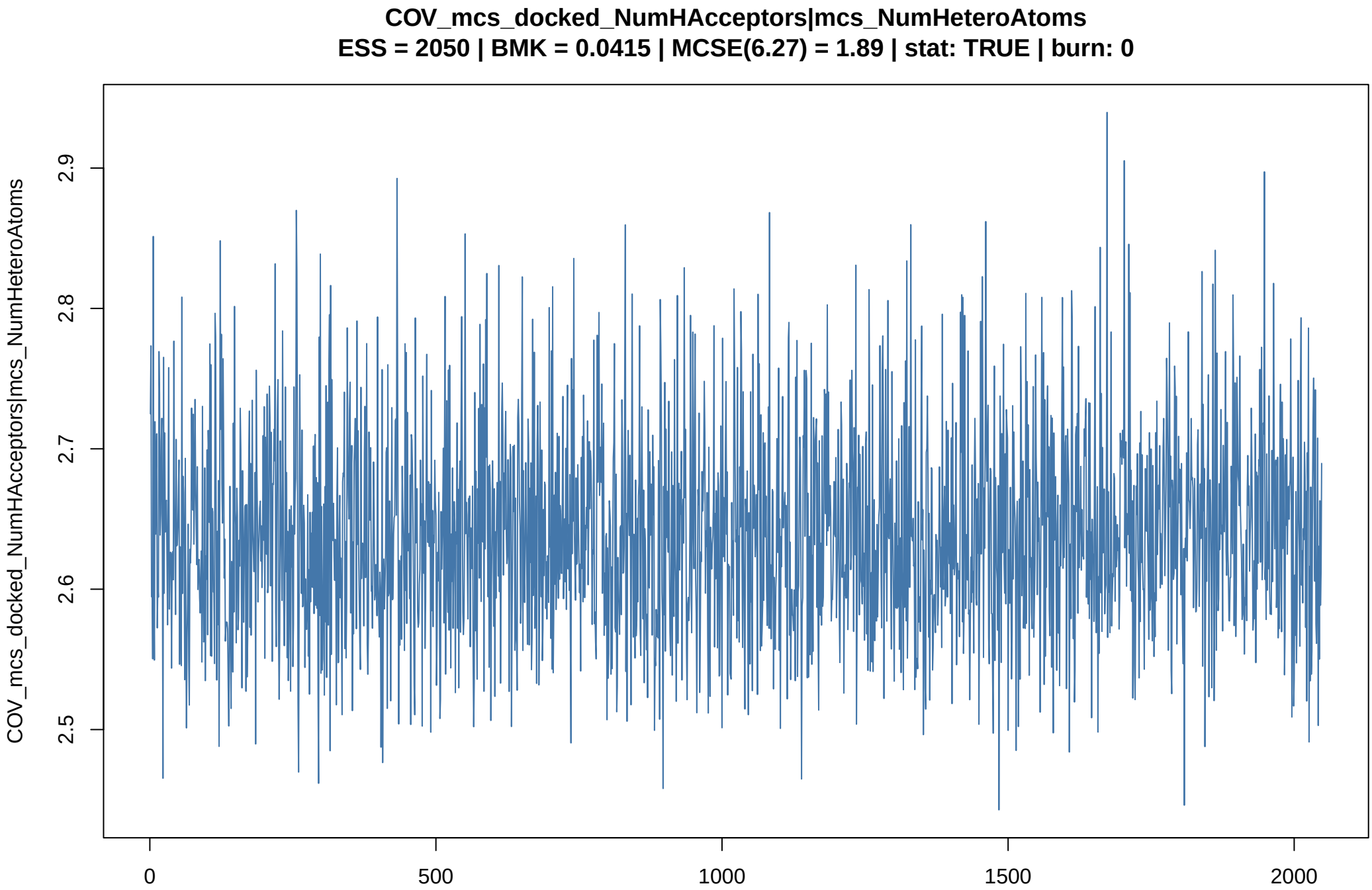

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2010 | BMK = 0.0549 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
0
500
1000
1500
2000

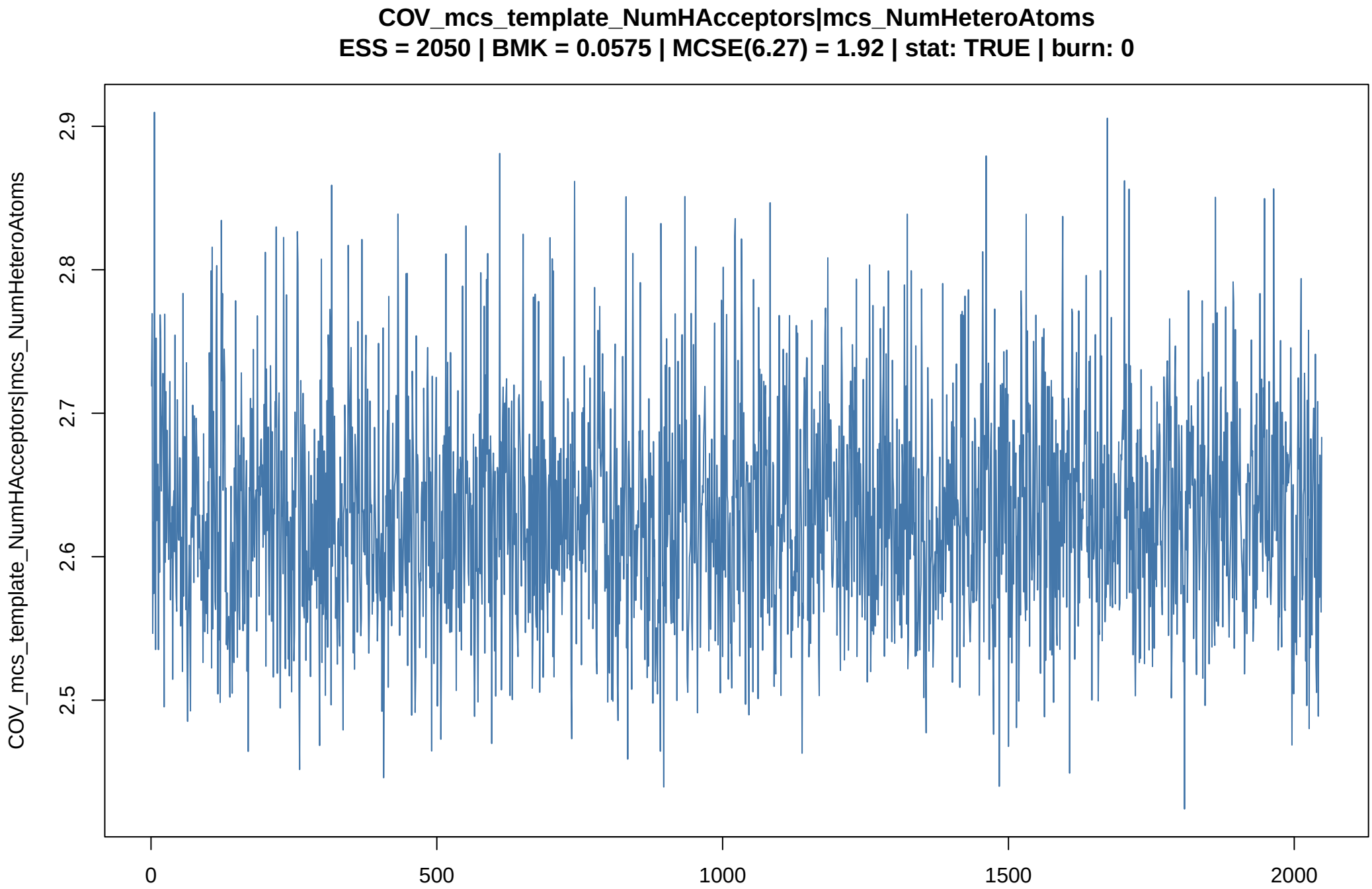

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1590 | BMK = 0.0407 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0428 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
0.8
0.6
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1730 | BMK = 0.0237 | MCSE(6.27) = 2.08 | stat: TRUE | 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 = 0.0483 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
1.9
2.0
2.1
2.2
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0415 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0575 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000