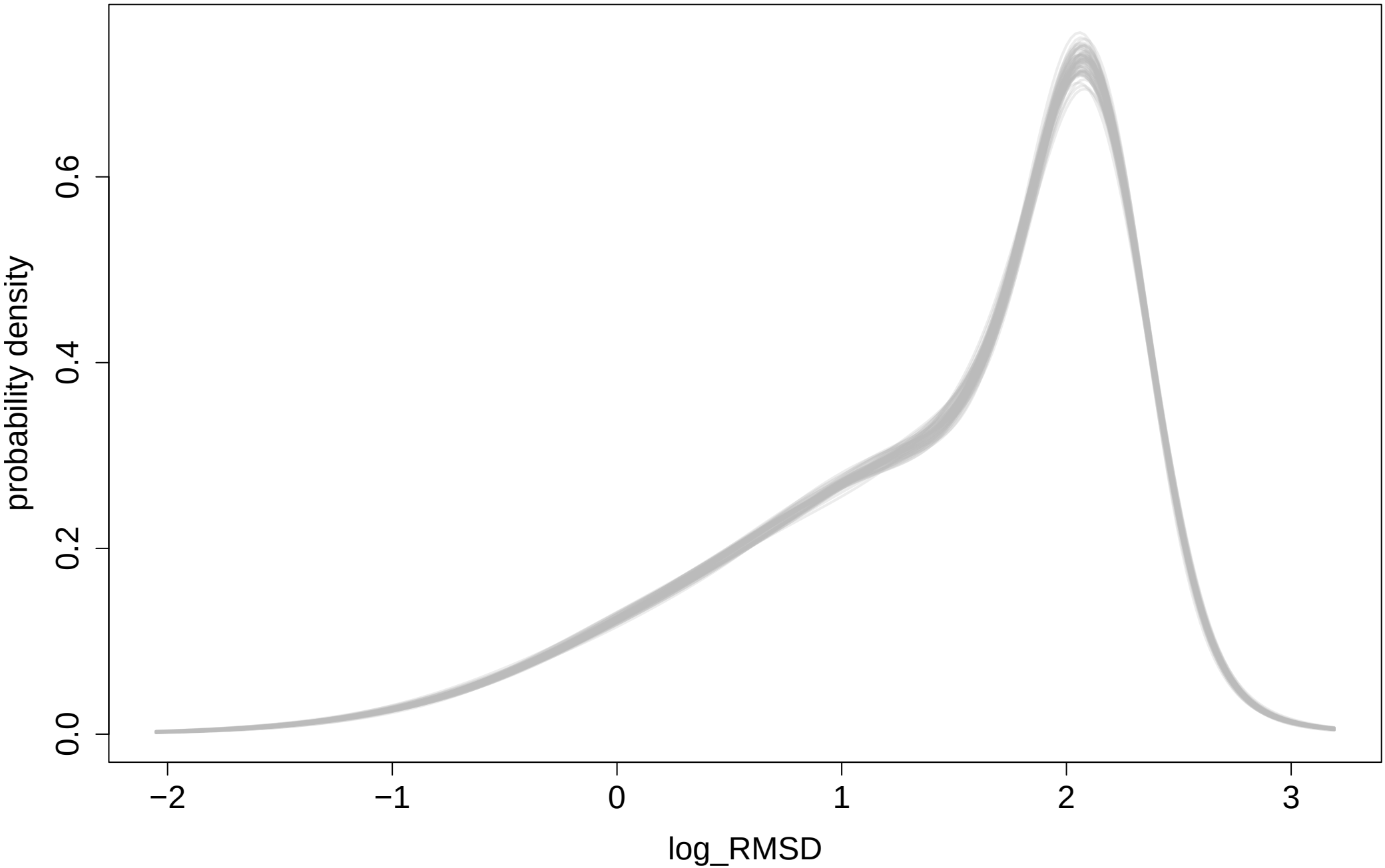
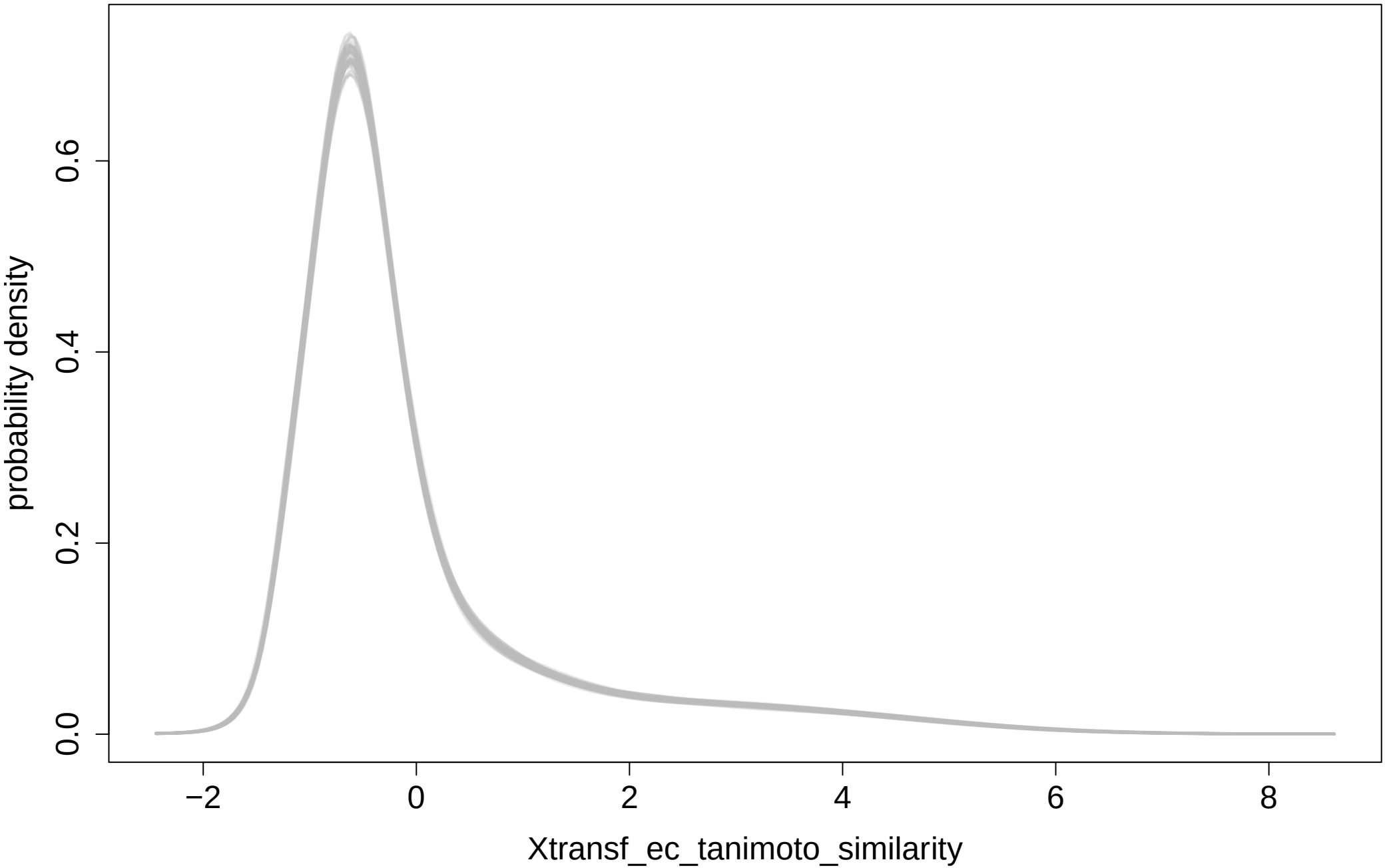
−− STATS maxD −−
min ESS = 2.7741904695483
max BMK = 0.73057619934581
max MCSE = 14.406454675271
all stationary: FALSE
burn: 2040

−− STATS 2D −−
min ESS = 1093.48776458908
max BMK = 0.080706778963435 4
max MCSE = 3.43106136302532
all stationary: FALSE
burn: 0

−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.758210958389277
max MCSE = NaN
all stationary: FALSE
burn: 2040

Occupied clusters: 66 of 91
LL: −110000 +− 102


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


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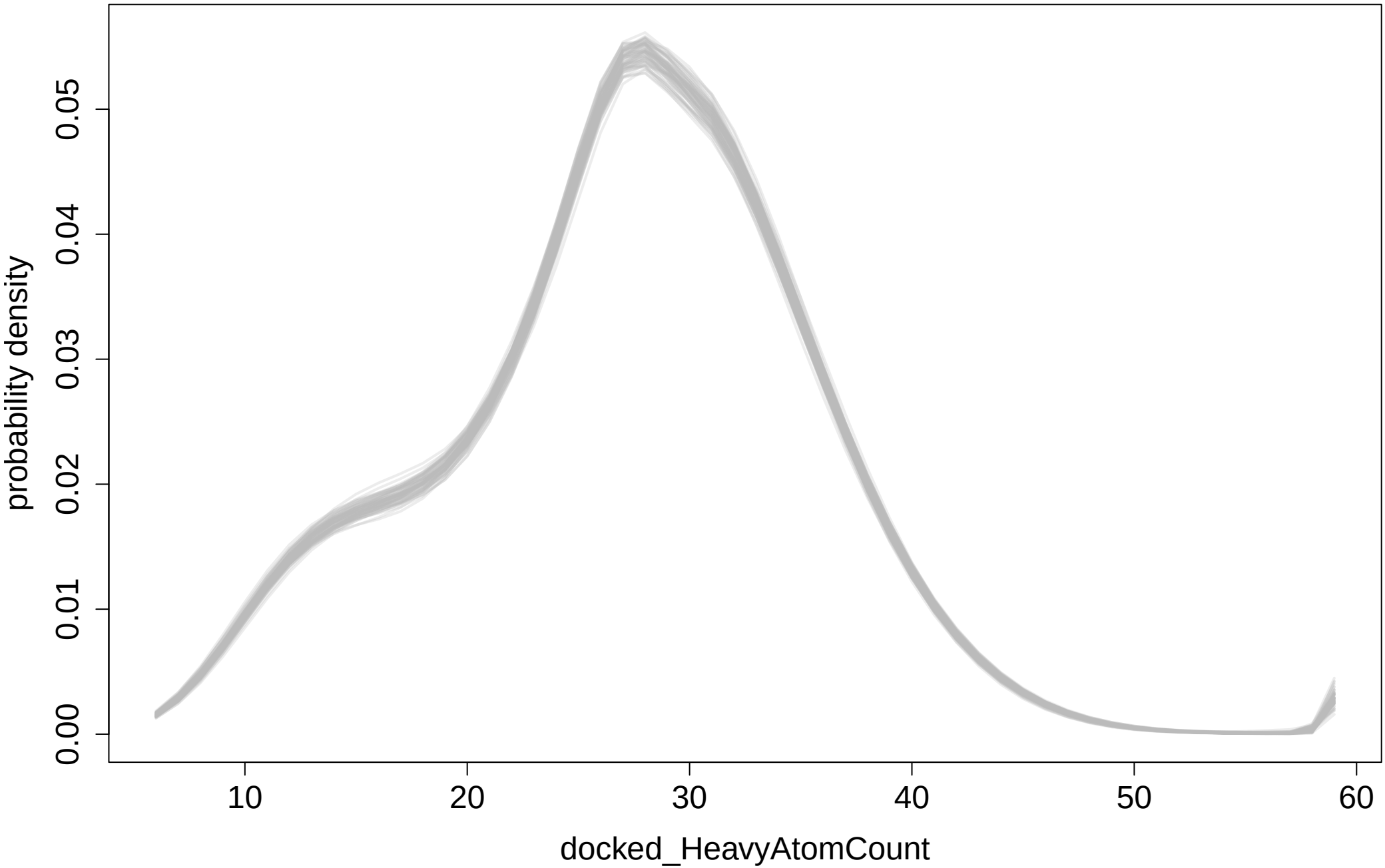
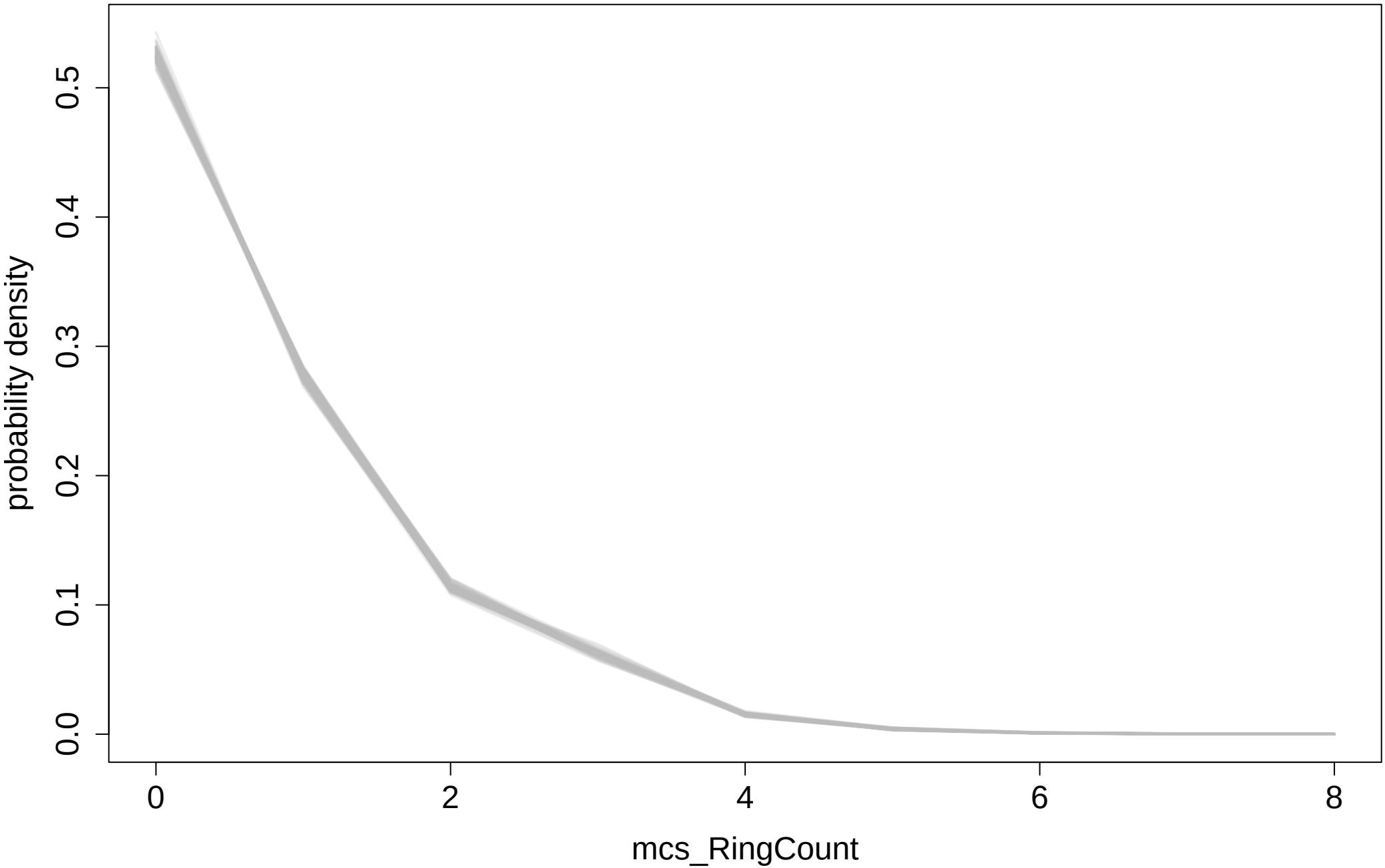
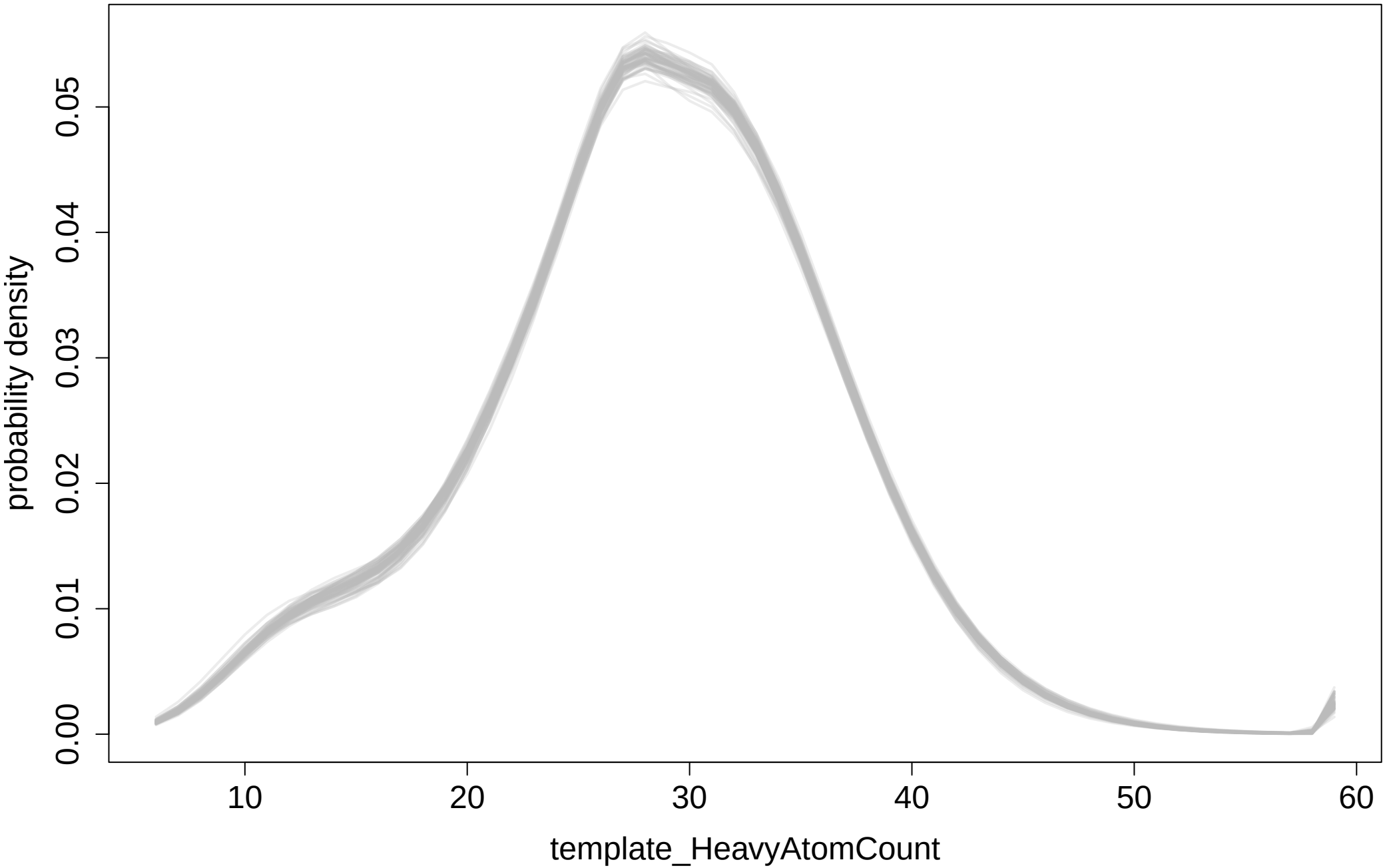
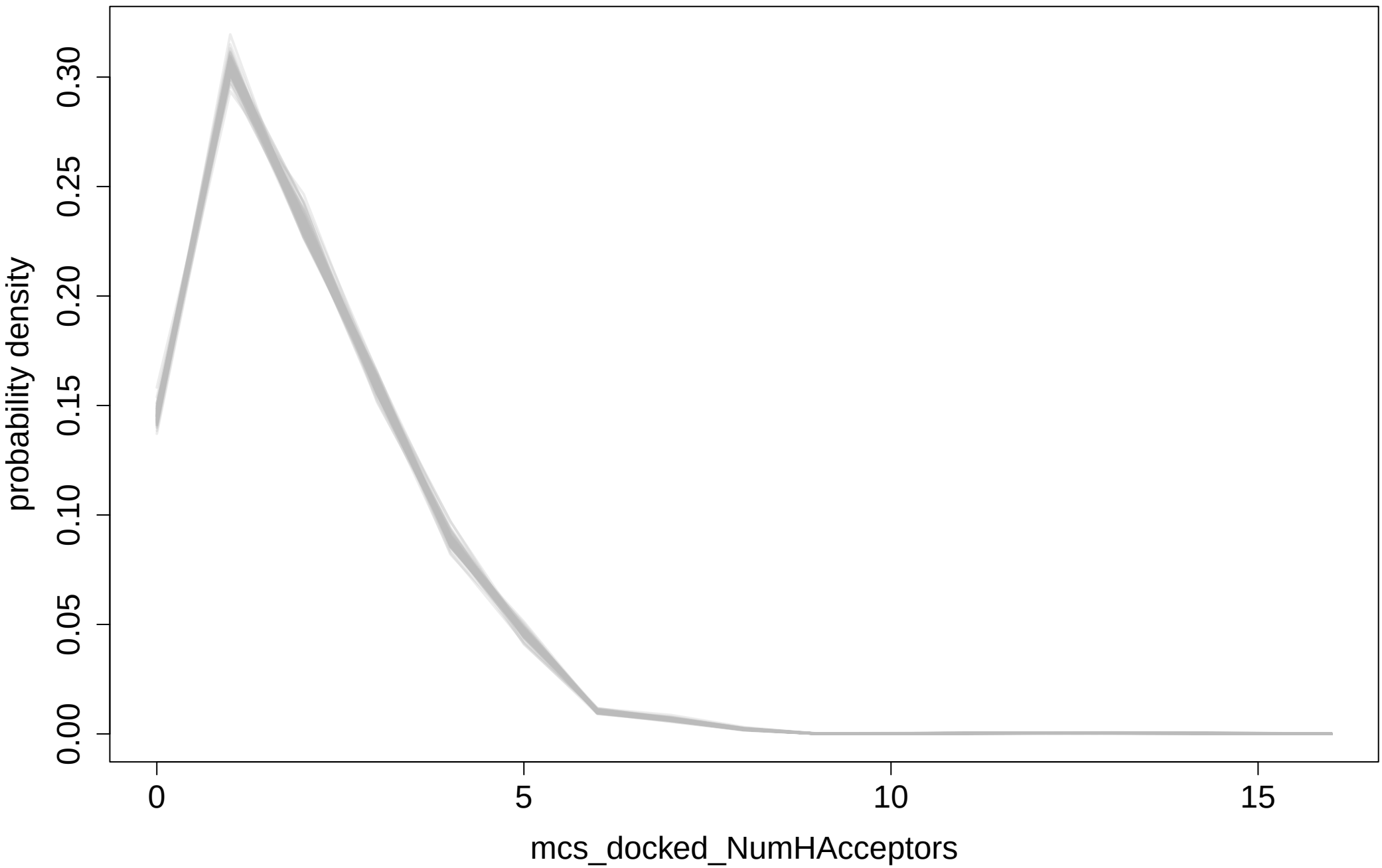
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity


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
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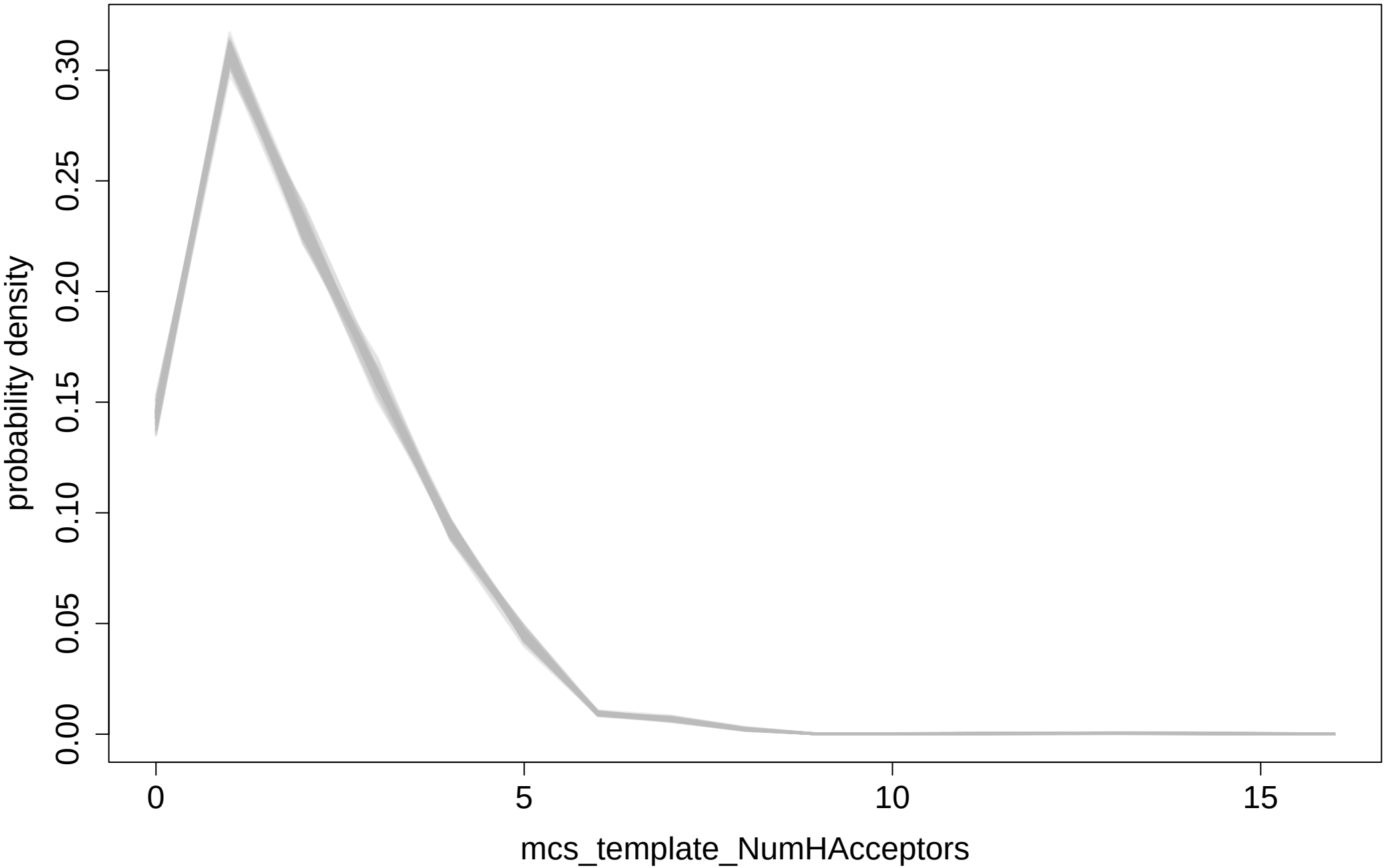
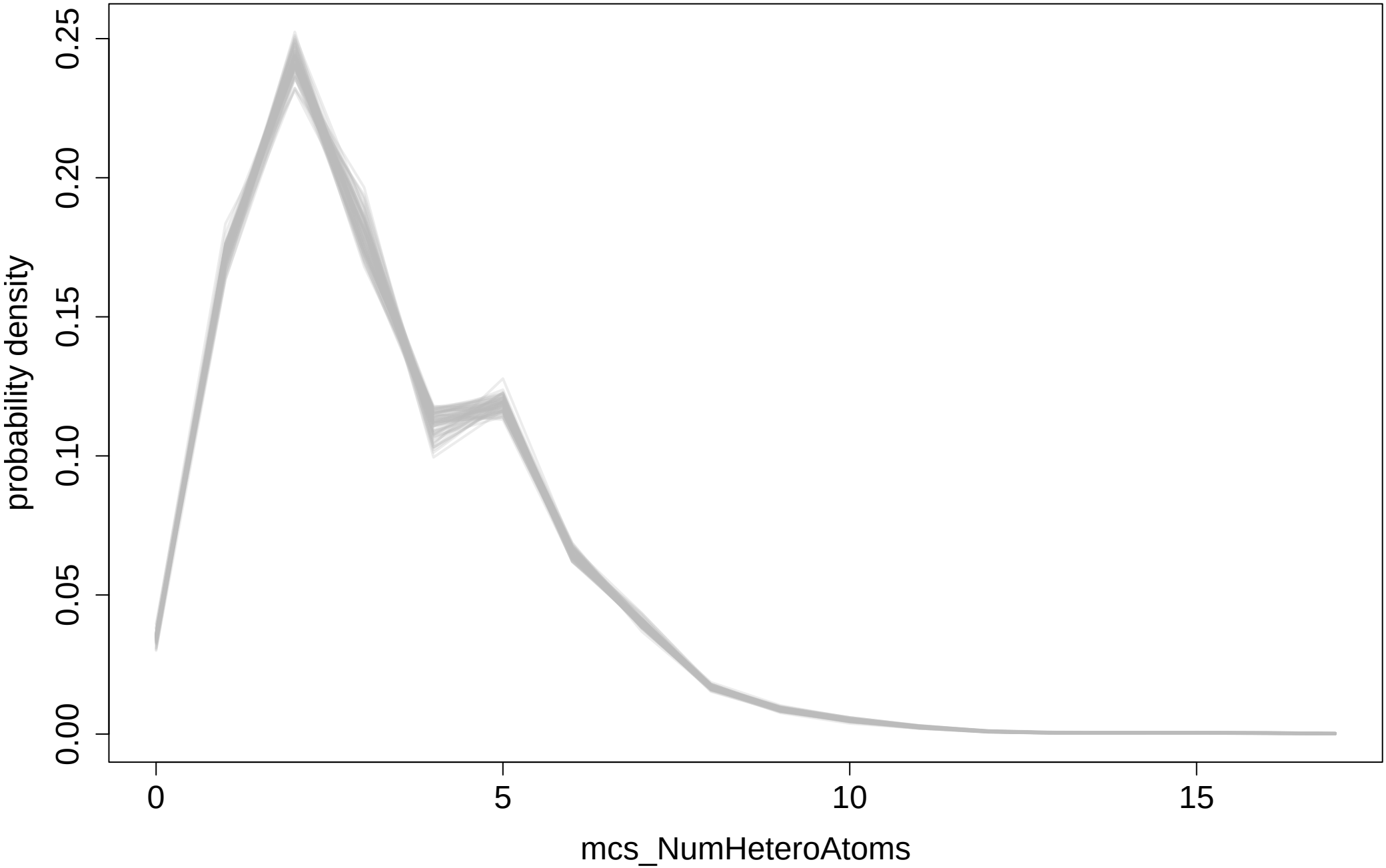
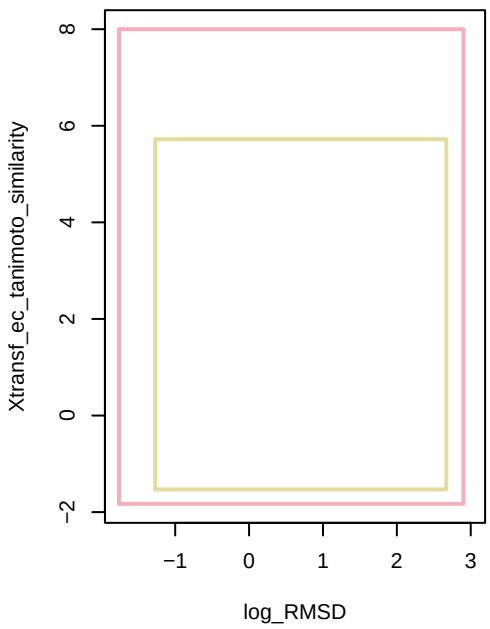
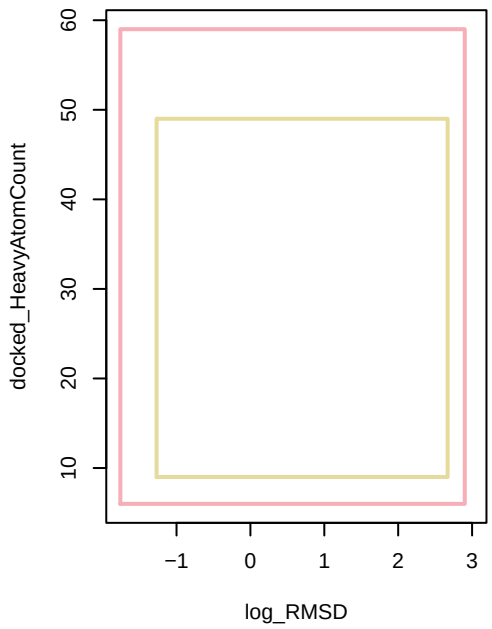
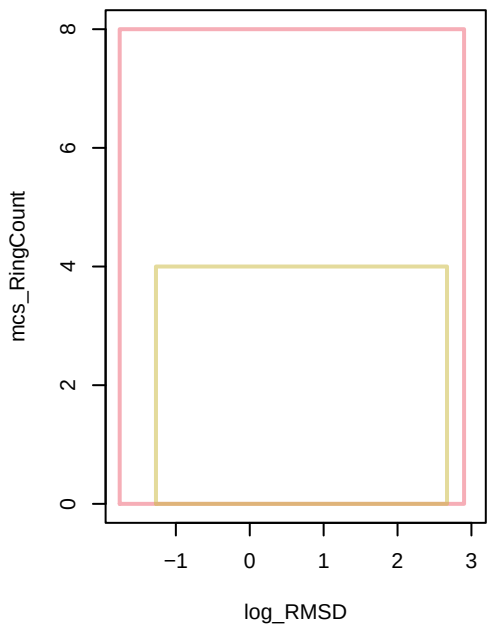
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

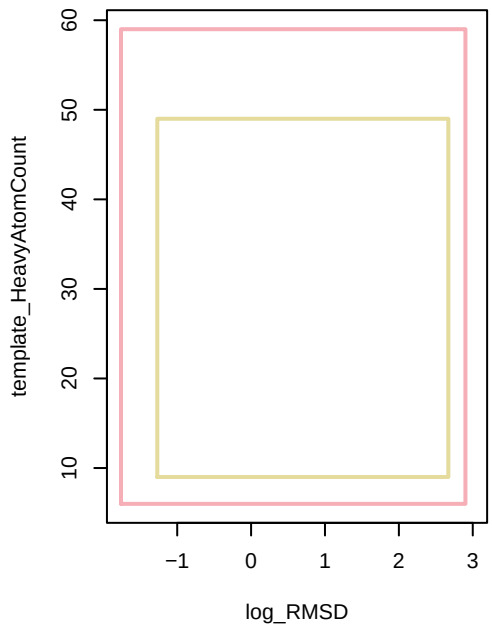

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

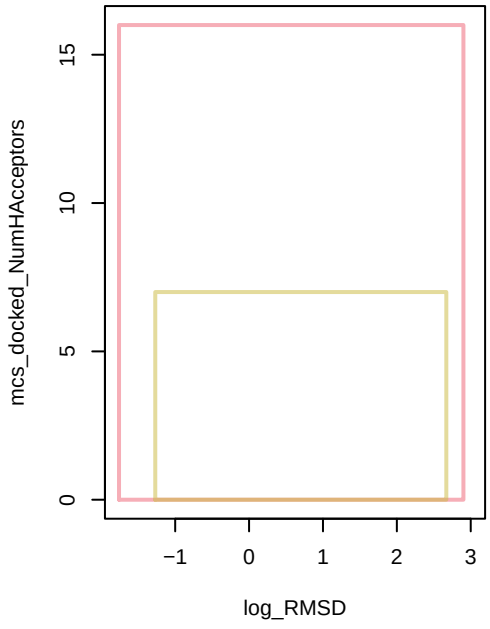

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

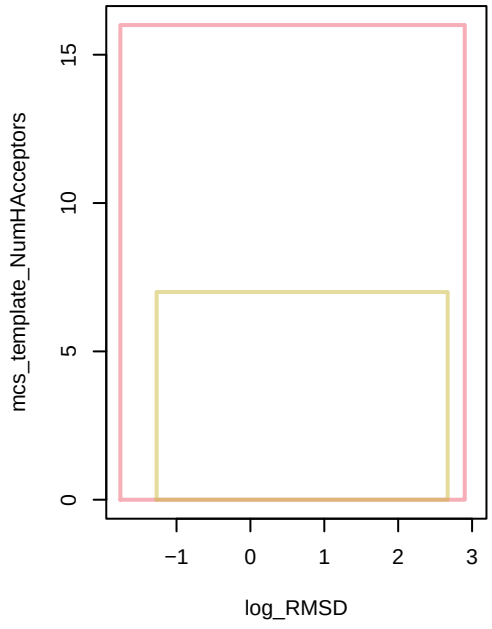

Xtransf_ec_tanimoto_similarity
log_RMSD

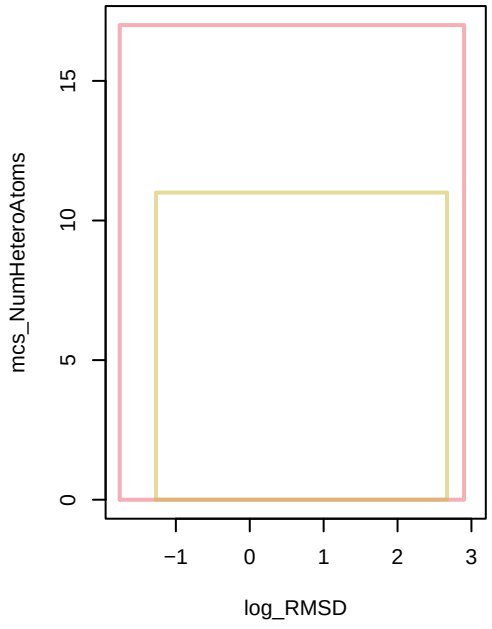

docked_HeavyAtomCount
log_RMSD

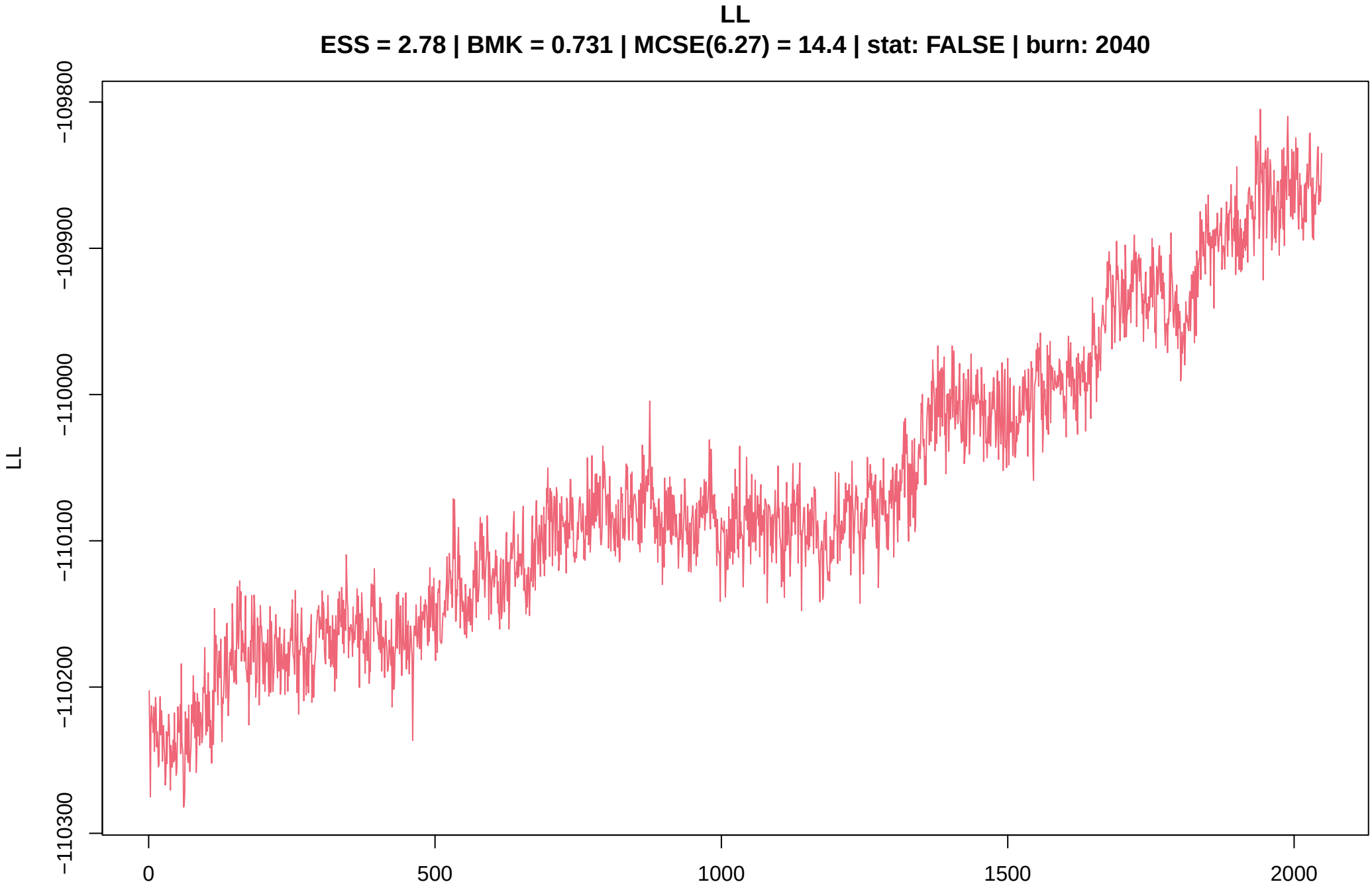

mcs_RingCount
log_RMSD

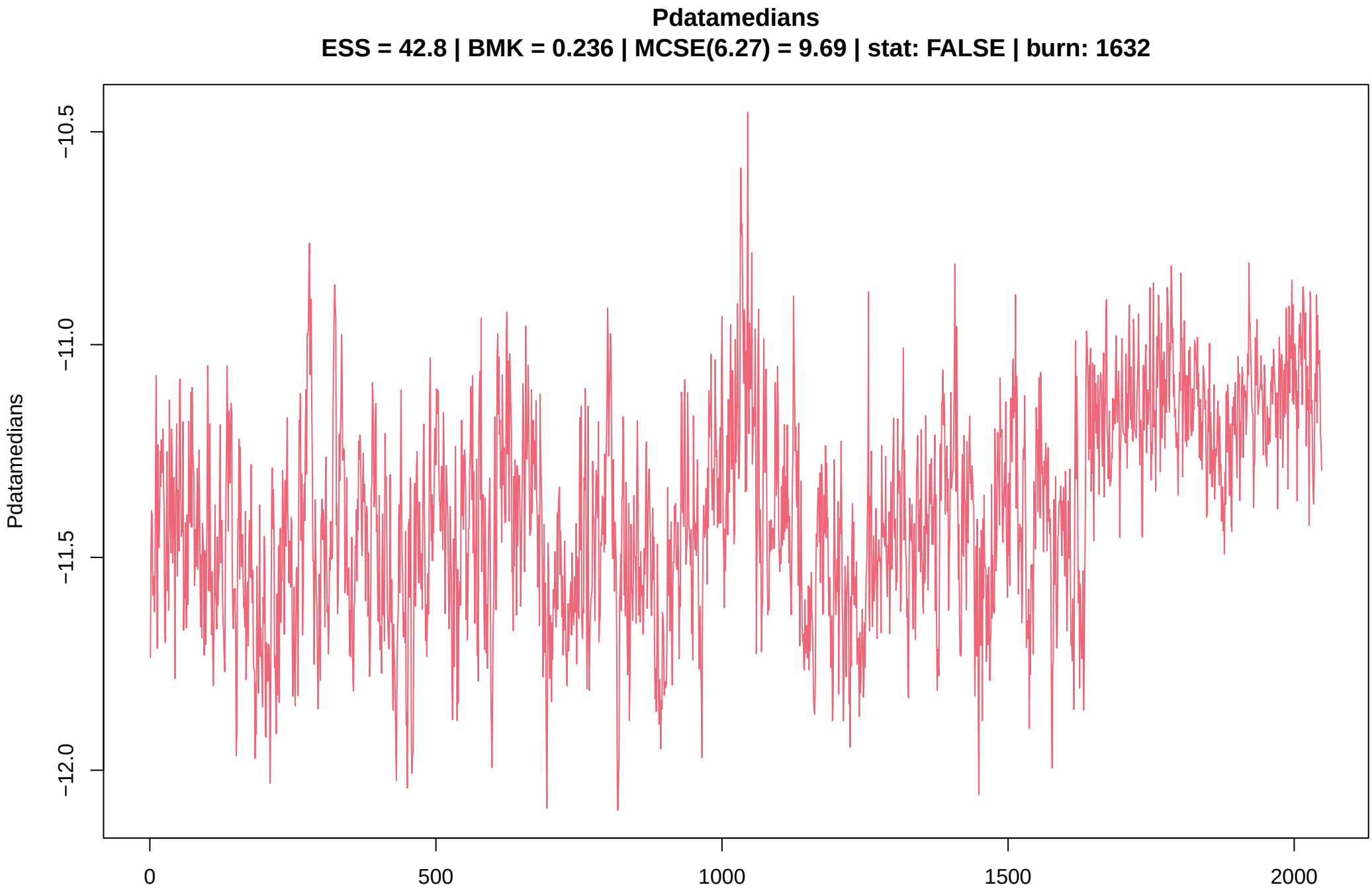

template_HeavyAtomCount
log_RMSD

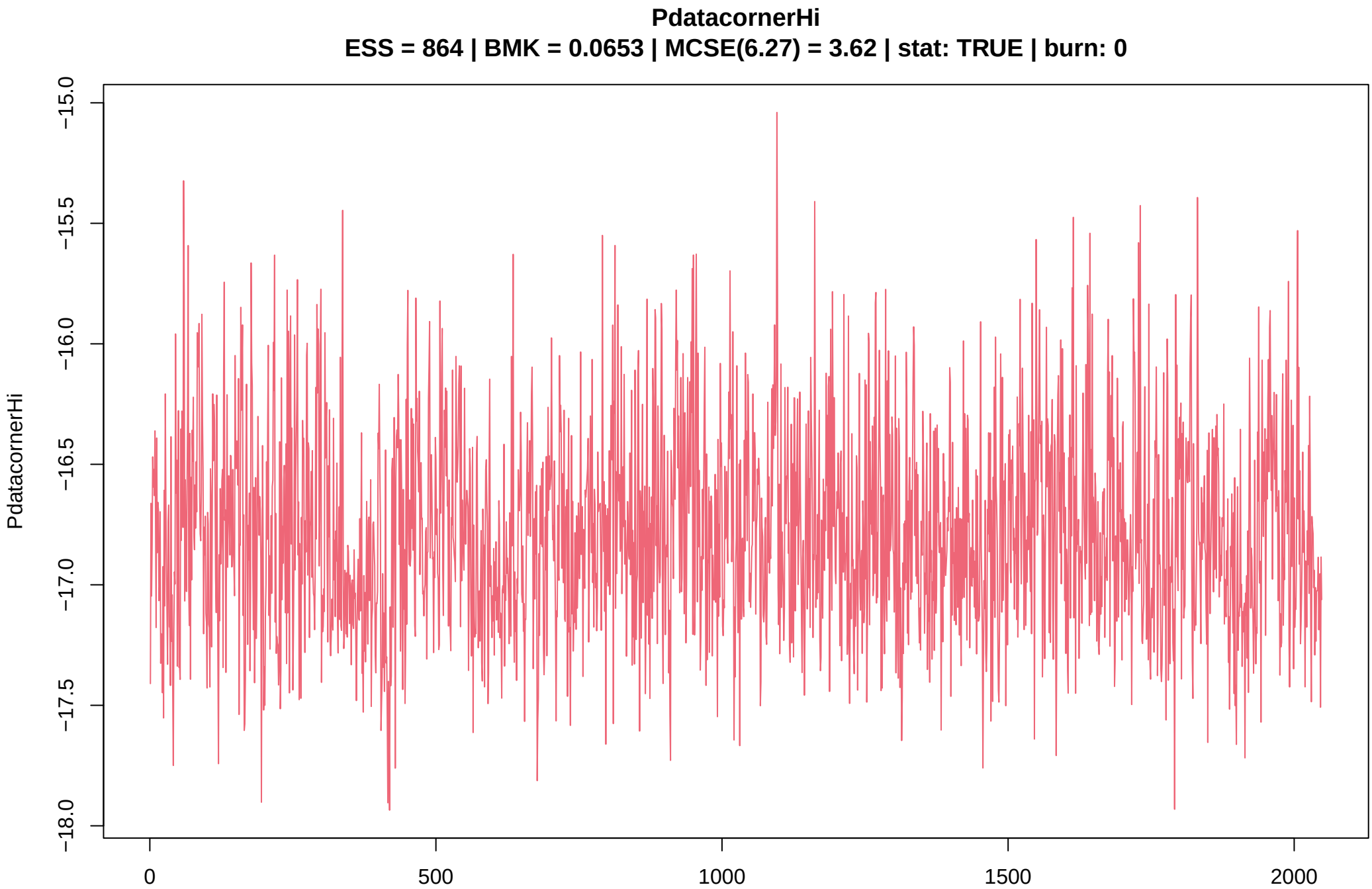

mcs_docked_NumHAcceptors
log_RMSD

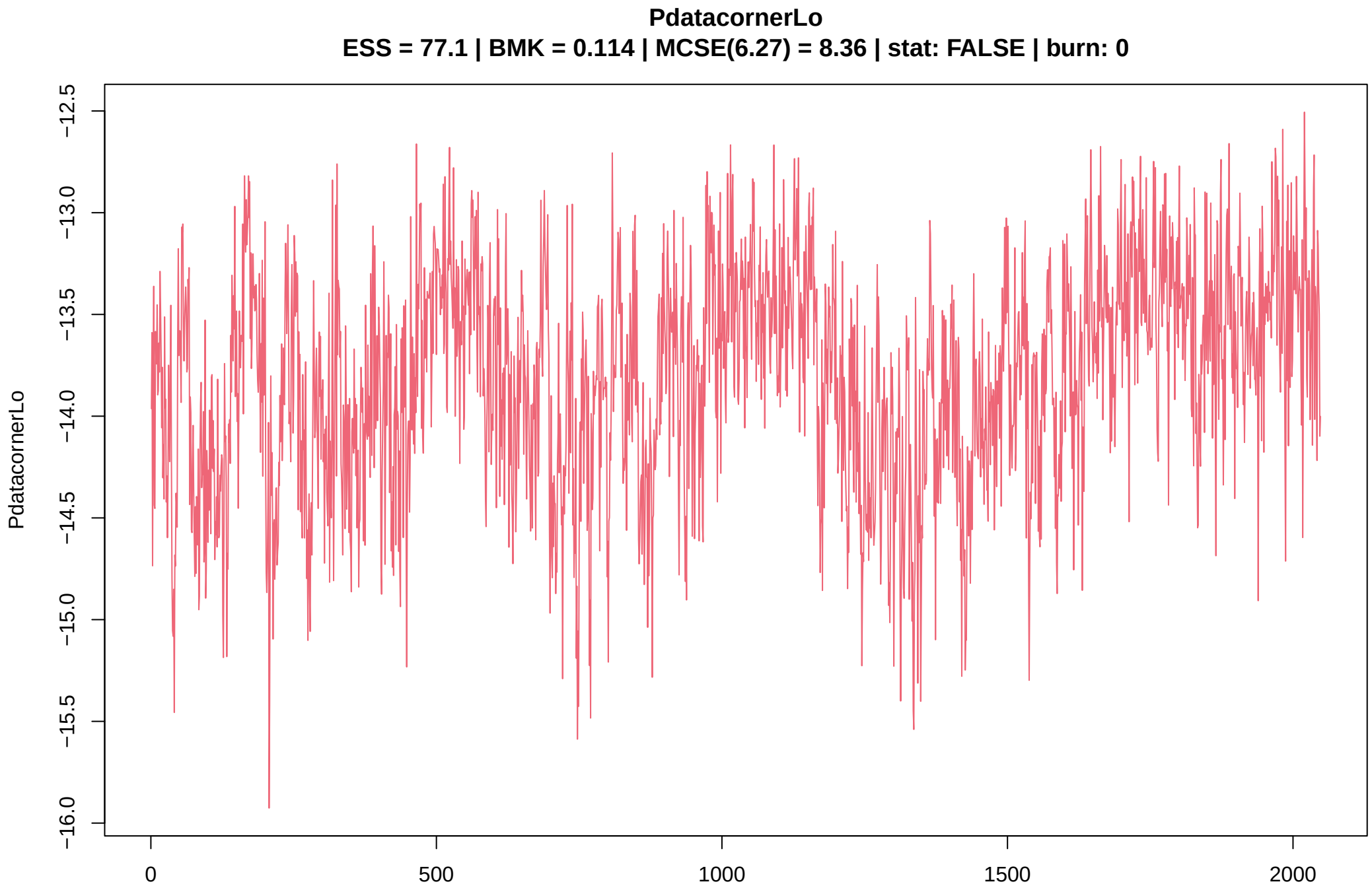

mcs_template_NumHAcceptors
log_RMSD

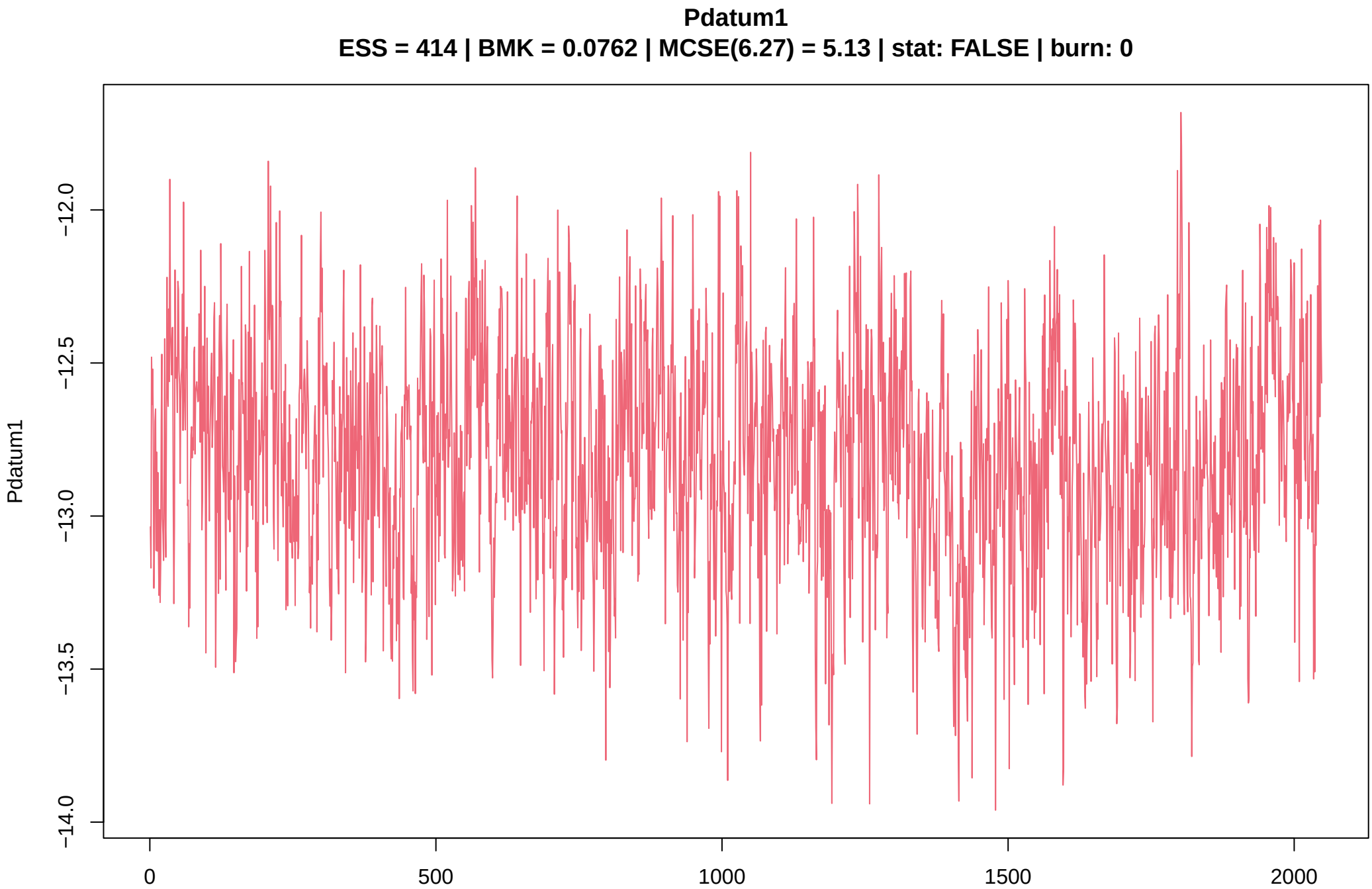

mcs_NumHeteroAtoms
log_RMSD

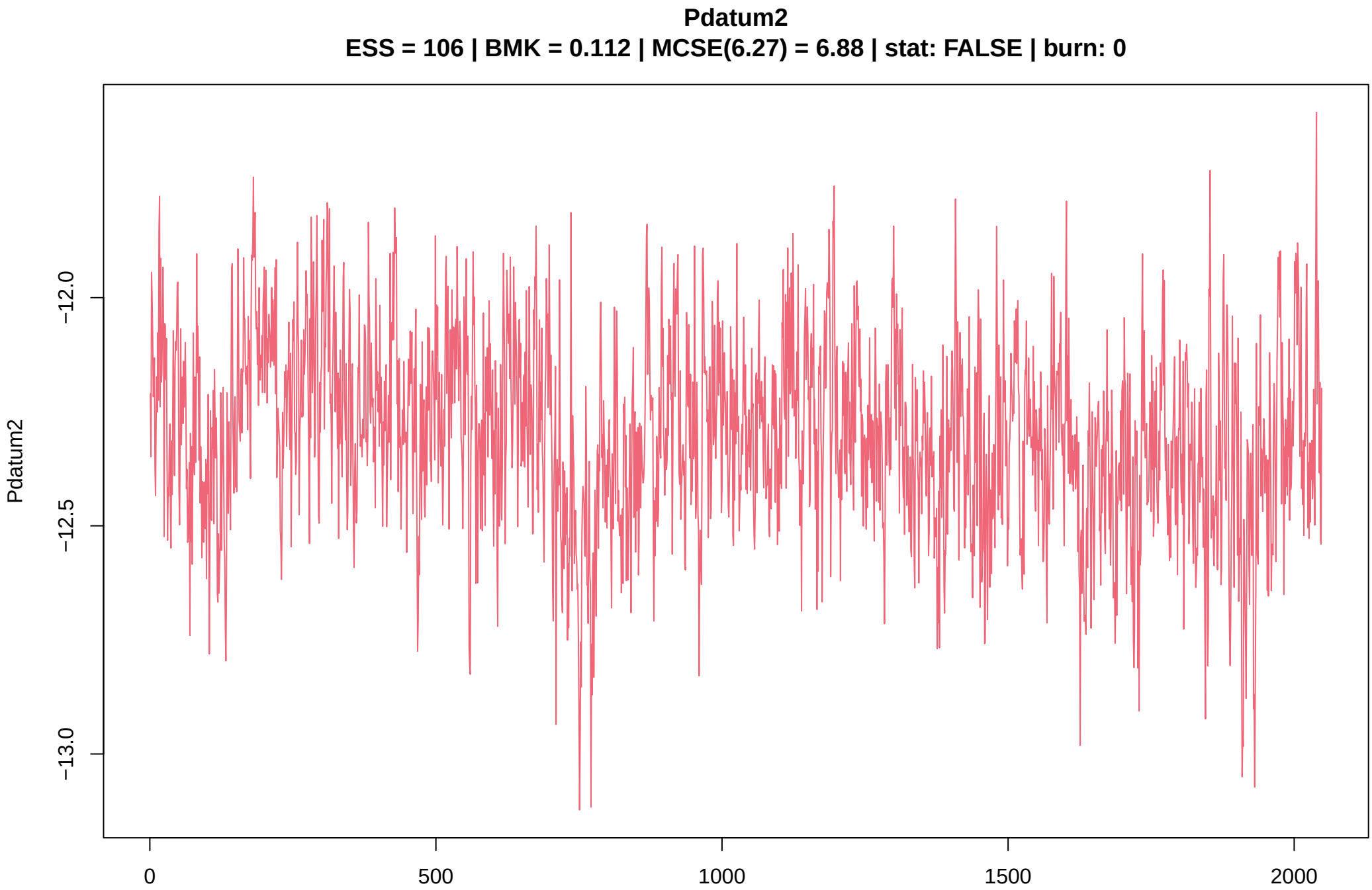

LL
ESS = 2.78 | BMK = 0.731 | MCSE(6.27) = 14.4 | stat: FALSE | burn: 2040
LL
−109800
−109900
−110000
−110100
−110200
−110300
0
500
1000
1500
2000

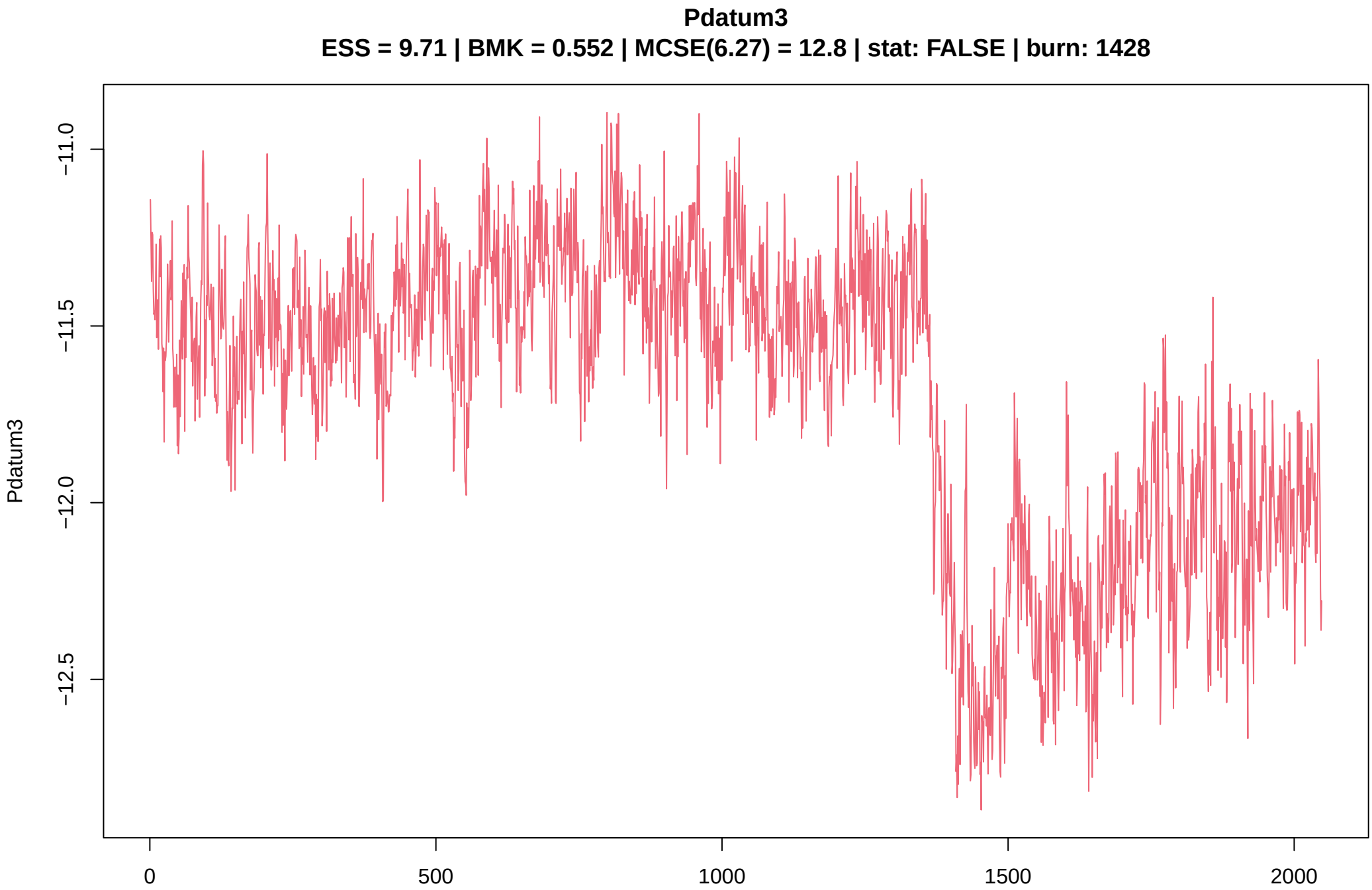

Pdatamedians
ESS = 42.8 | BMK = 0.236 | MCSE(6.27) = 9.69 | stat: FALSE | burn: 1632
Pdatamedians
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

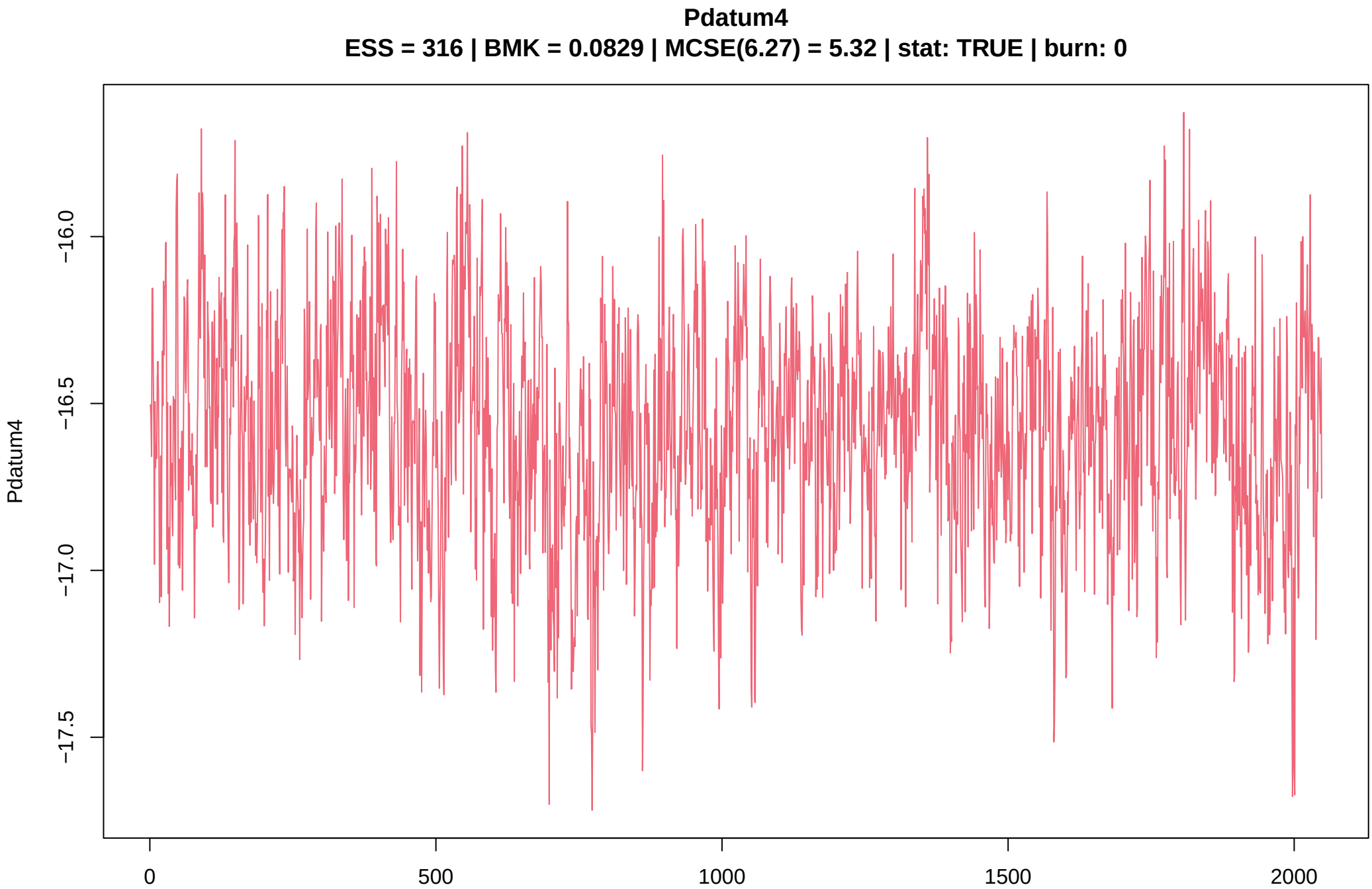

PdatacornerHi
ESS = 864 | BMK = 0.0653 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0
PdatacornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

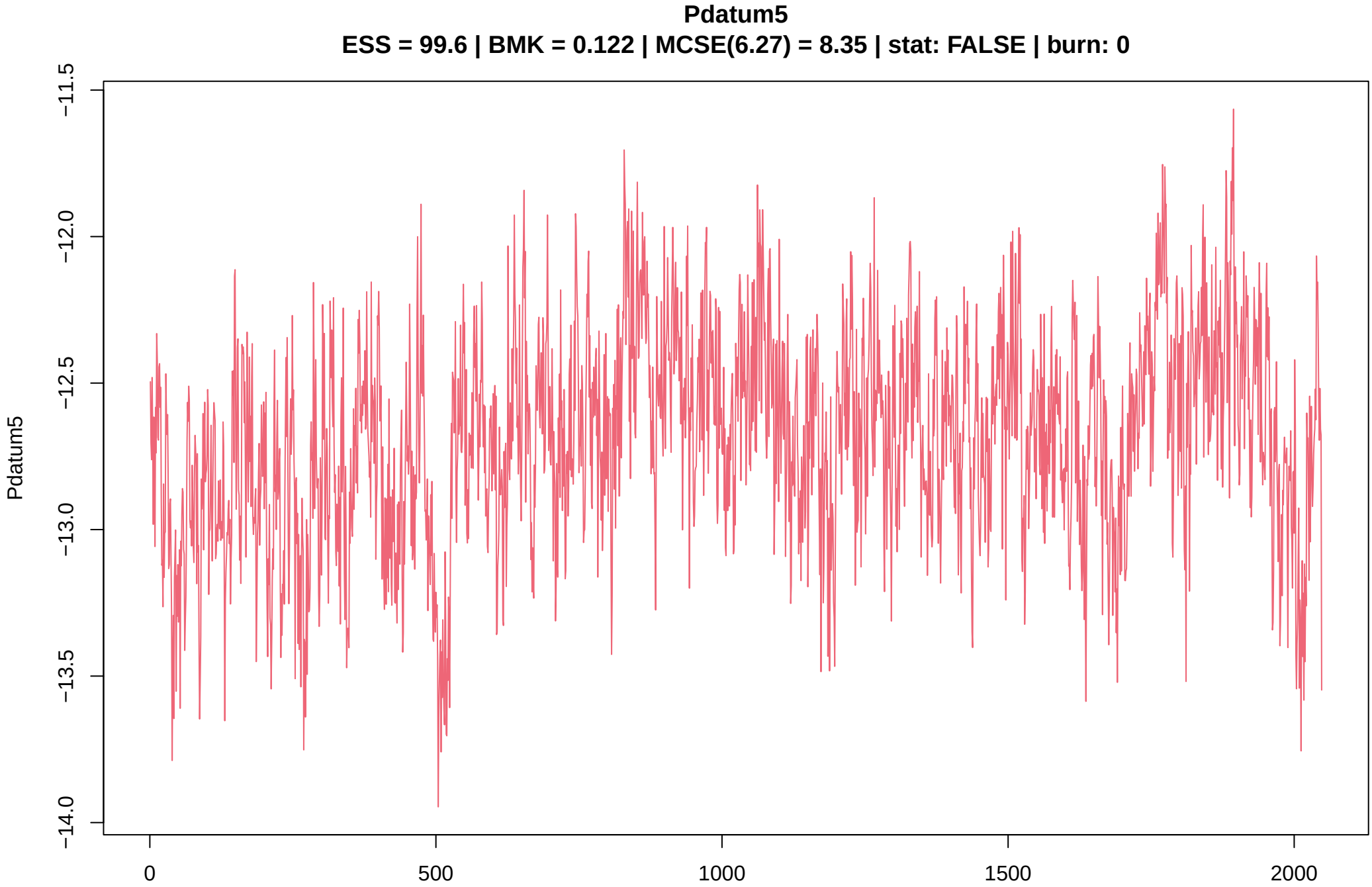

PdatacornerLo
ESS = 77.1 | BMK = 0.114 | MCSE(6.27) = 8.36 | stat: FALSE | burn: 0
PdatacornerLo
−12.5
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
0
500
1000
1500
2000

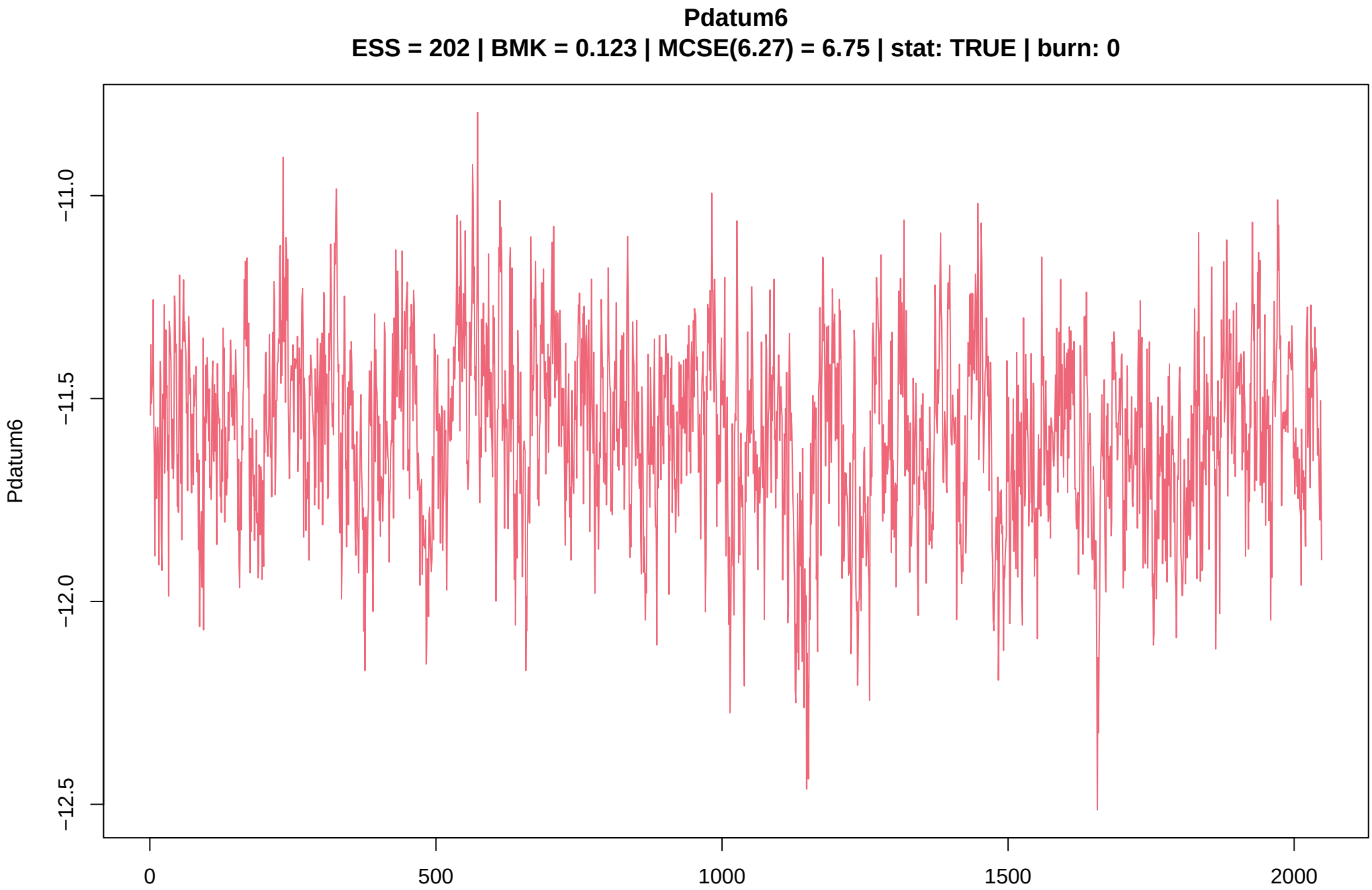

Pdatum1
ESS = 414 | BMK = 0.0762 | MCSE(6.27) = 5.13 | stat: FALSE | burn: 0
Pdatum1
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

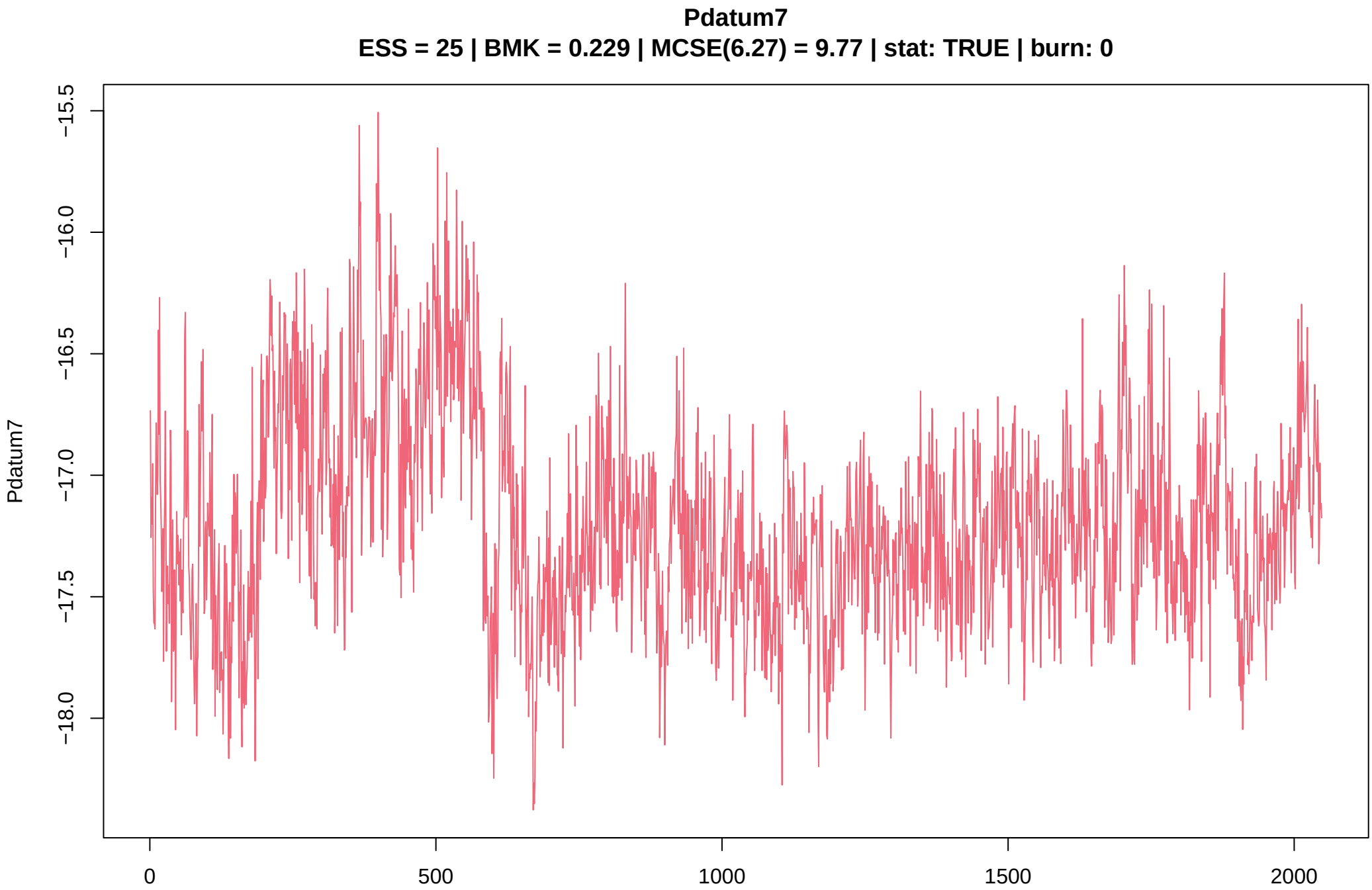

Pdatum2
ESS = 106 | BMK = 0.112 | MCSE(6.27) = 6.88 | stat: FALSE | burn: 0
Pdatum2
−12.0
−12.5
−13.0
0
500
1000
1500
2000

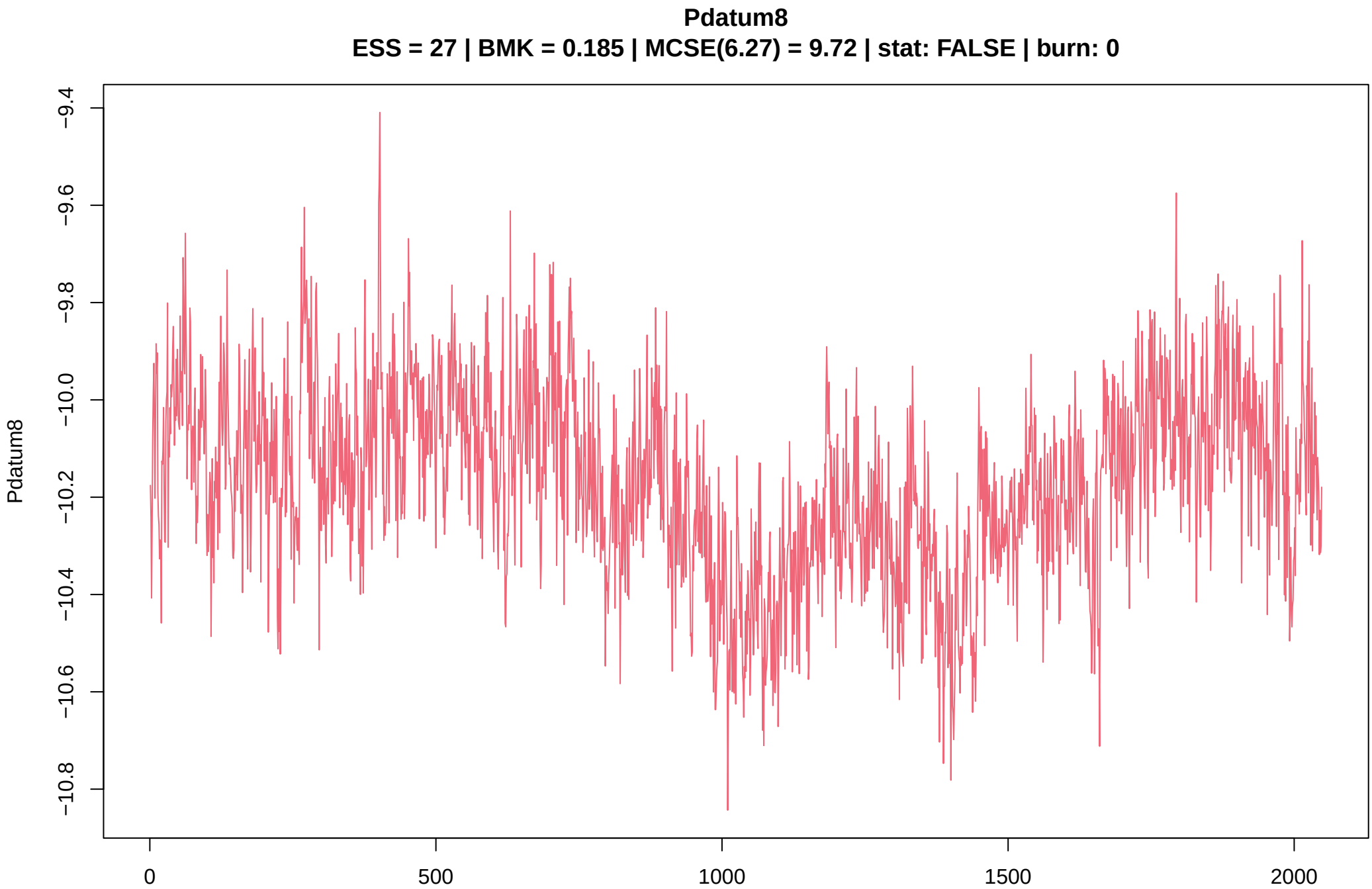

Pdatum3
ESS = 9.71 | BMK = 0.552 | MCSE(6.27) = 12.8 | stat: FALSE | burn: 1428
Pdatum3
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

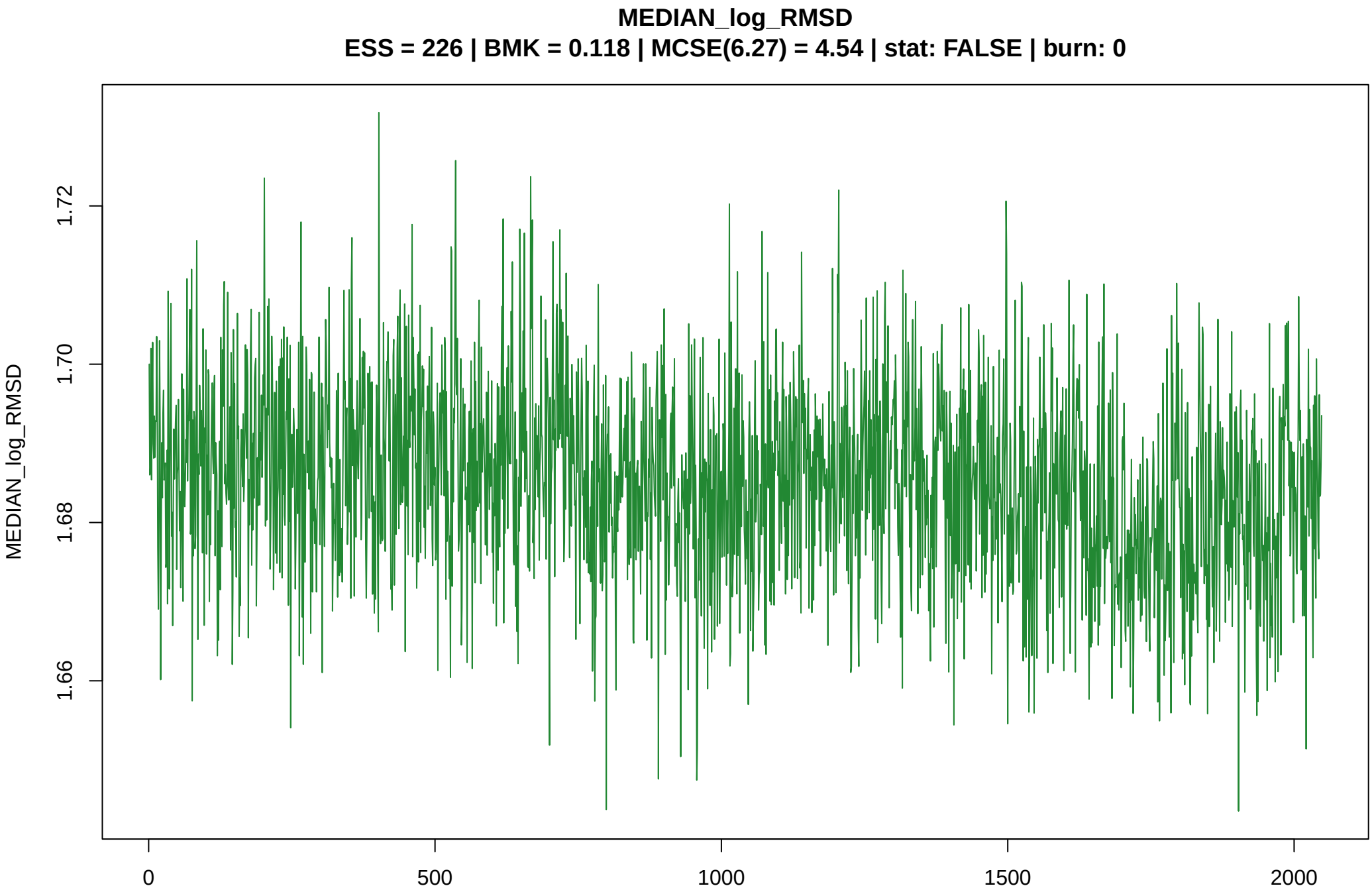

Pdatum4
ESS = 316 | BMK = 0.0829 | MCSE(6.27) = 5.32 | stat: TRUE | burn: 0
Pdatum4
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

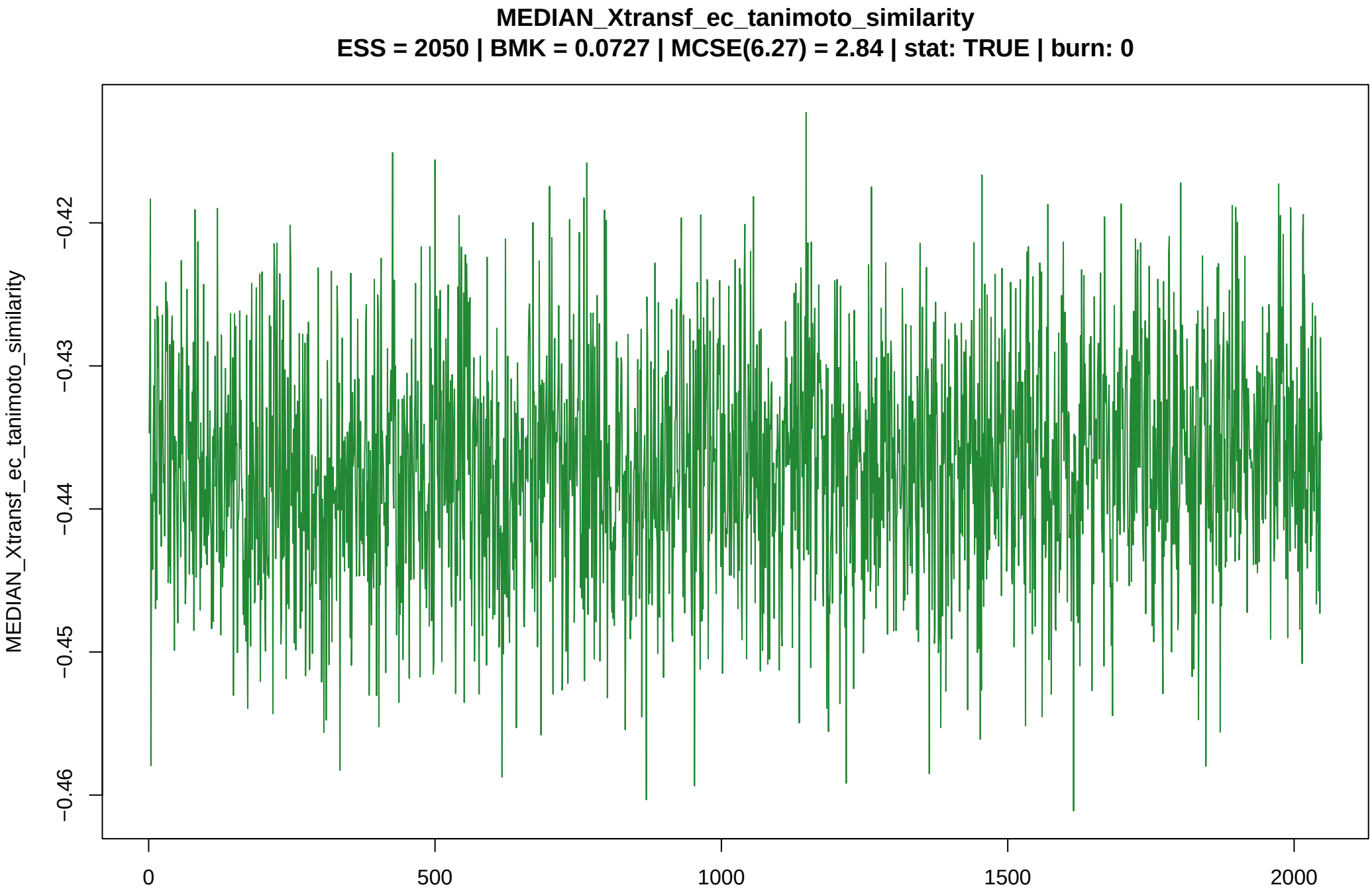

Pdatum5
ESS = 99.6 | BMK = 0.122 | MCSE(6.27) = 8.35 | stat: FALSE | burn: 0
Pdatum5
−11.5
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

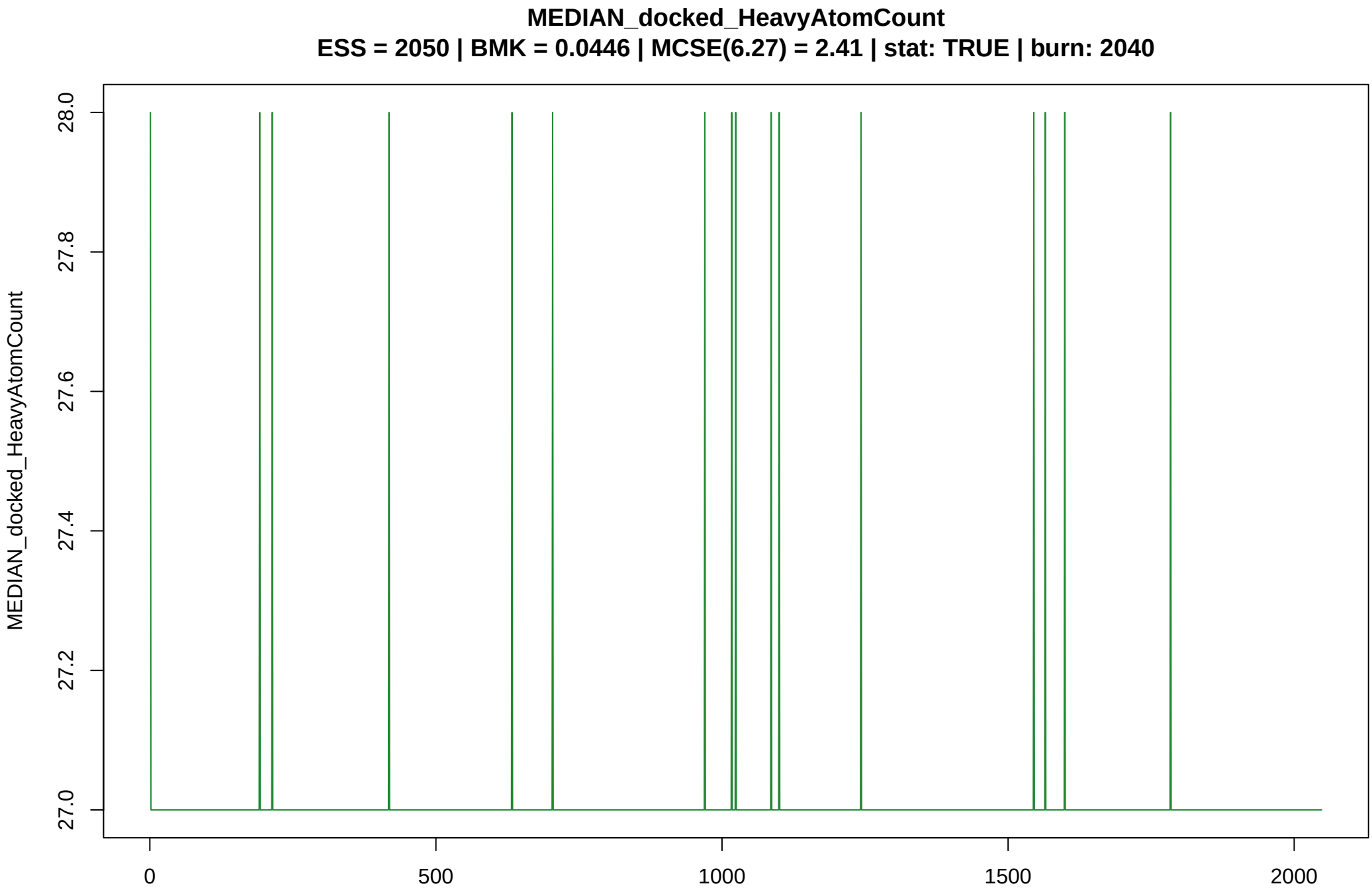

Pdatum6
ESS = 202 | BMK = 0.123 | MCSE(6.27) = 6.75 | stat: TRUE | burn: 0
Pdatum6
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

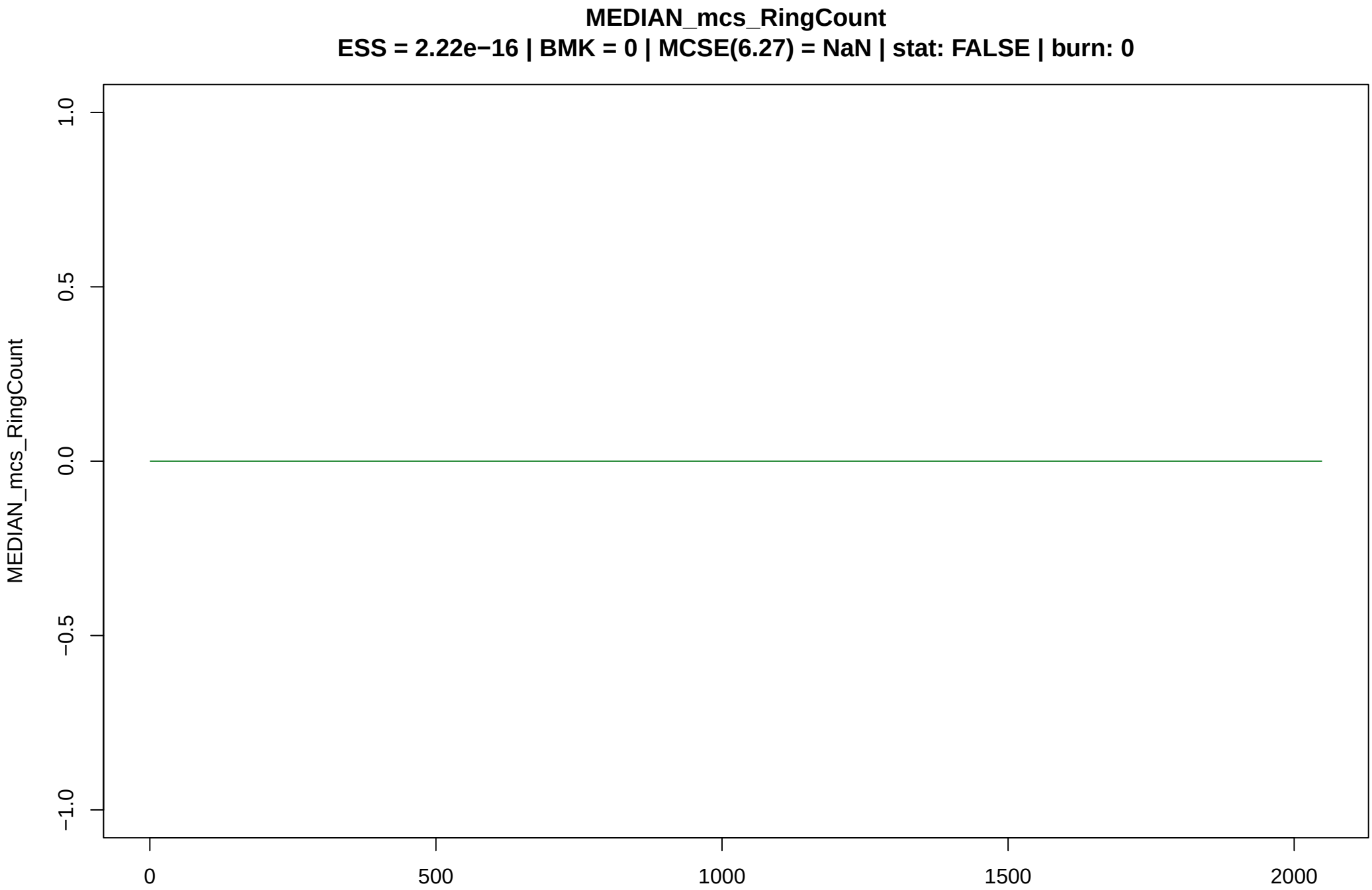

Pdatum7
ESS = 25 | BMK = 0.229 | MCSE(6.27) = 9.77 | stat: TRUE | burn: 0
Pdatum7
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

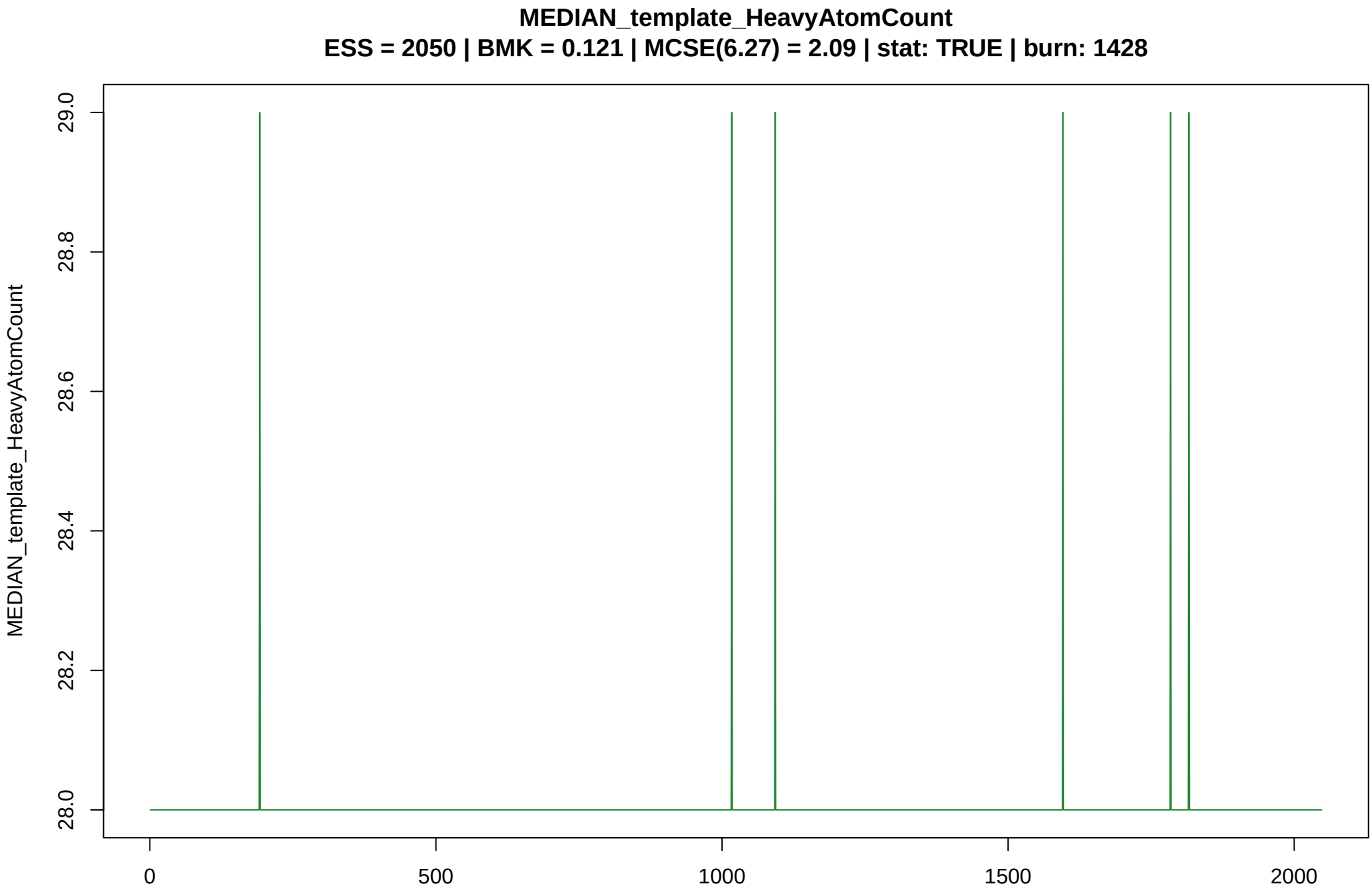

Pdatum8
ESS = 27 | BMK = 0.185 | MCSE(6.27) = 9.72 | stat: FALSE | burn: 0
Pdatum8
−9.4
−9.6
−9.8
−10.0
−10.2
−10.4
−10.6
−10.8
0
500
1000
1500
2000

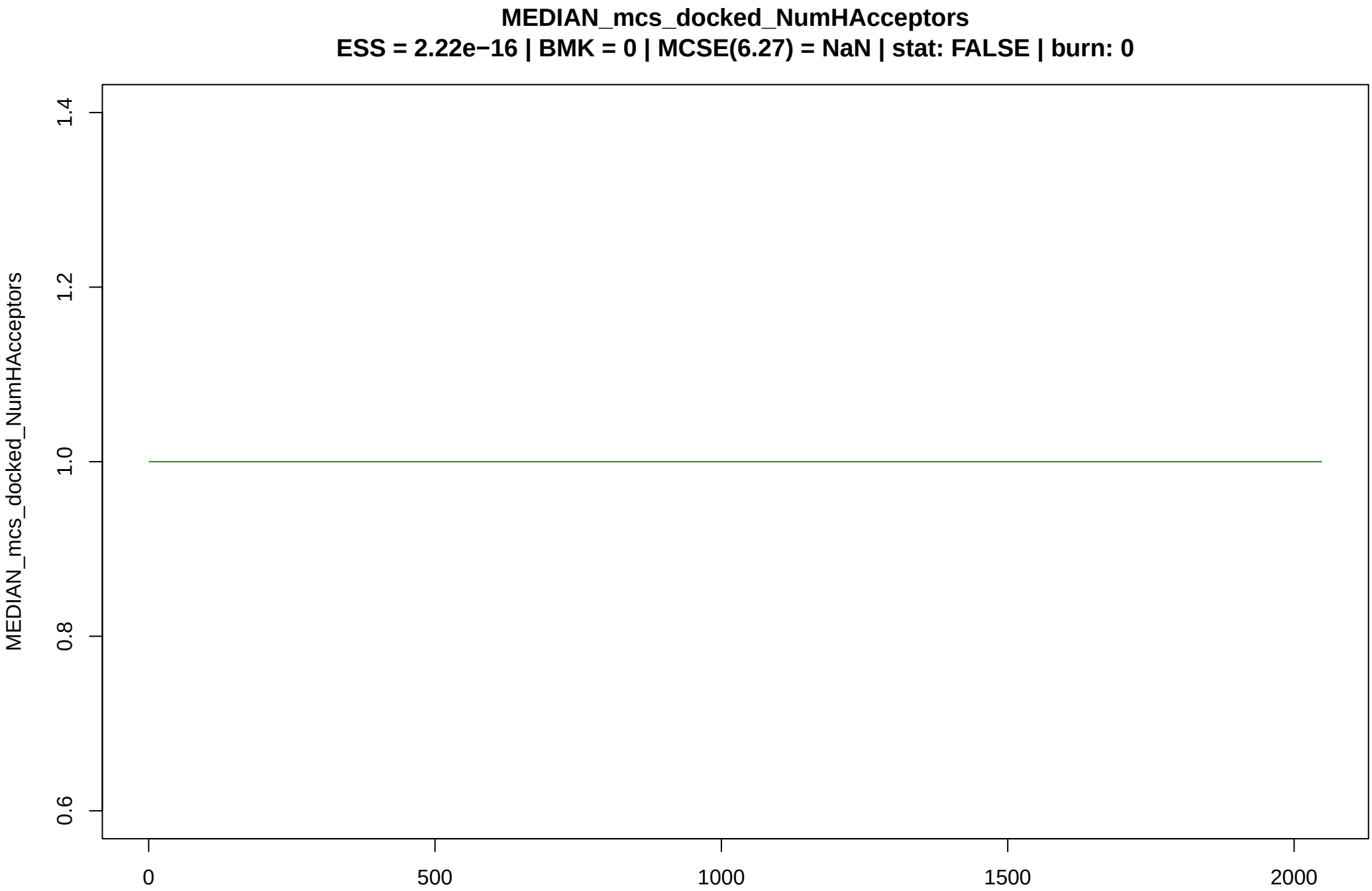

MEDIAN_log_RMSD
ESS = 226 | BMK = 0.118 | MCSE(6.27) = 4.54 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

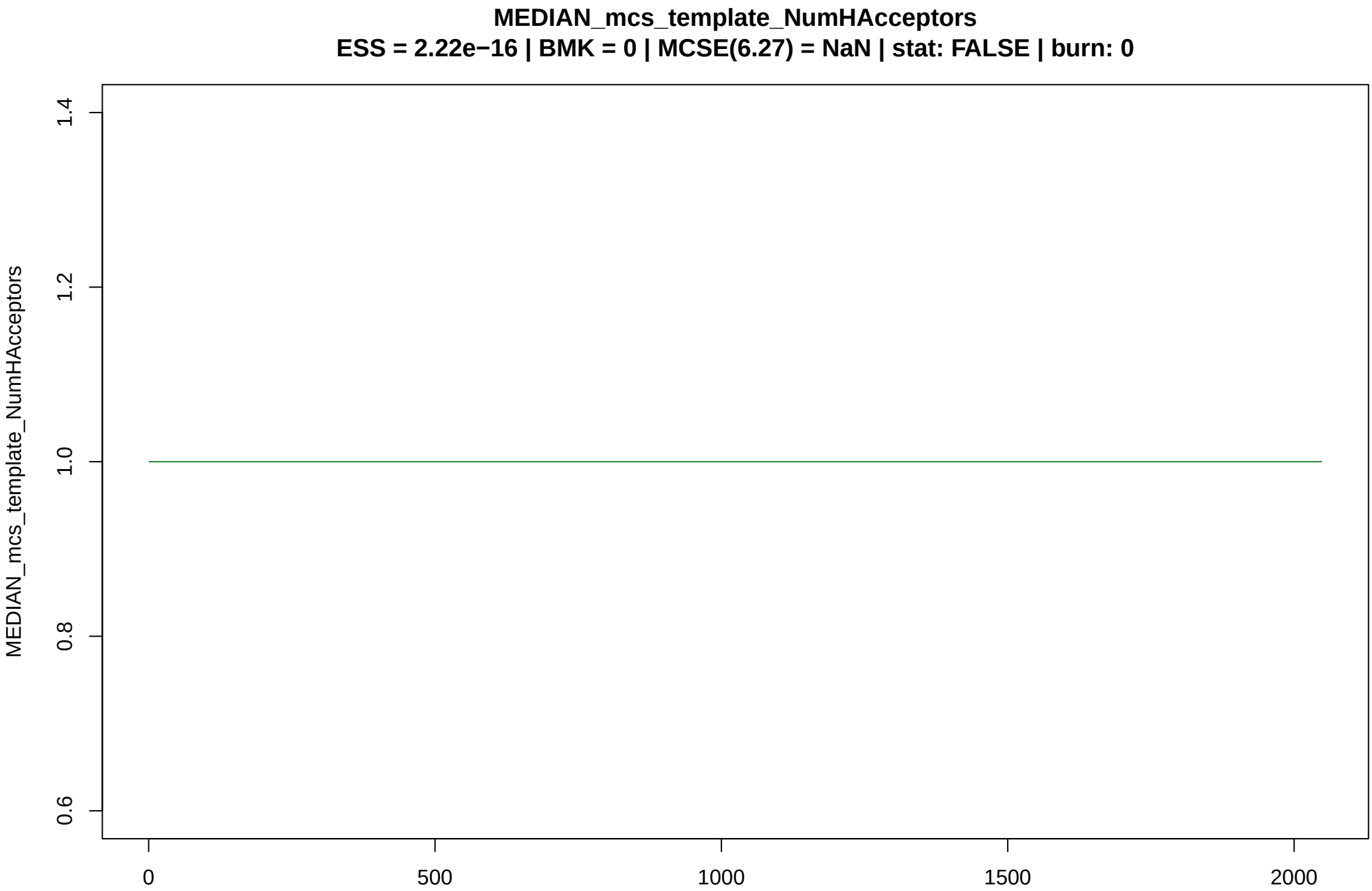

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0727 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

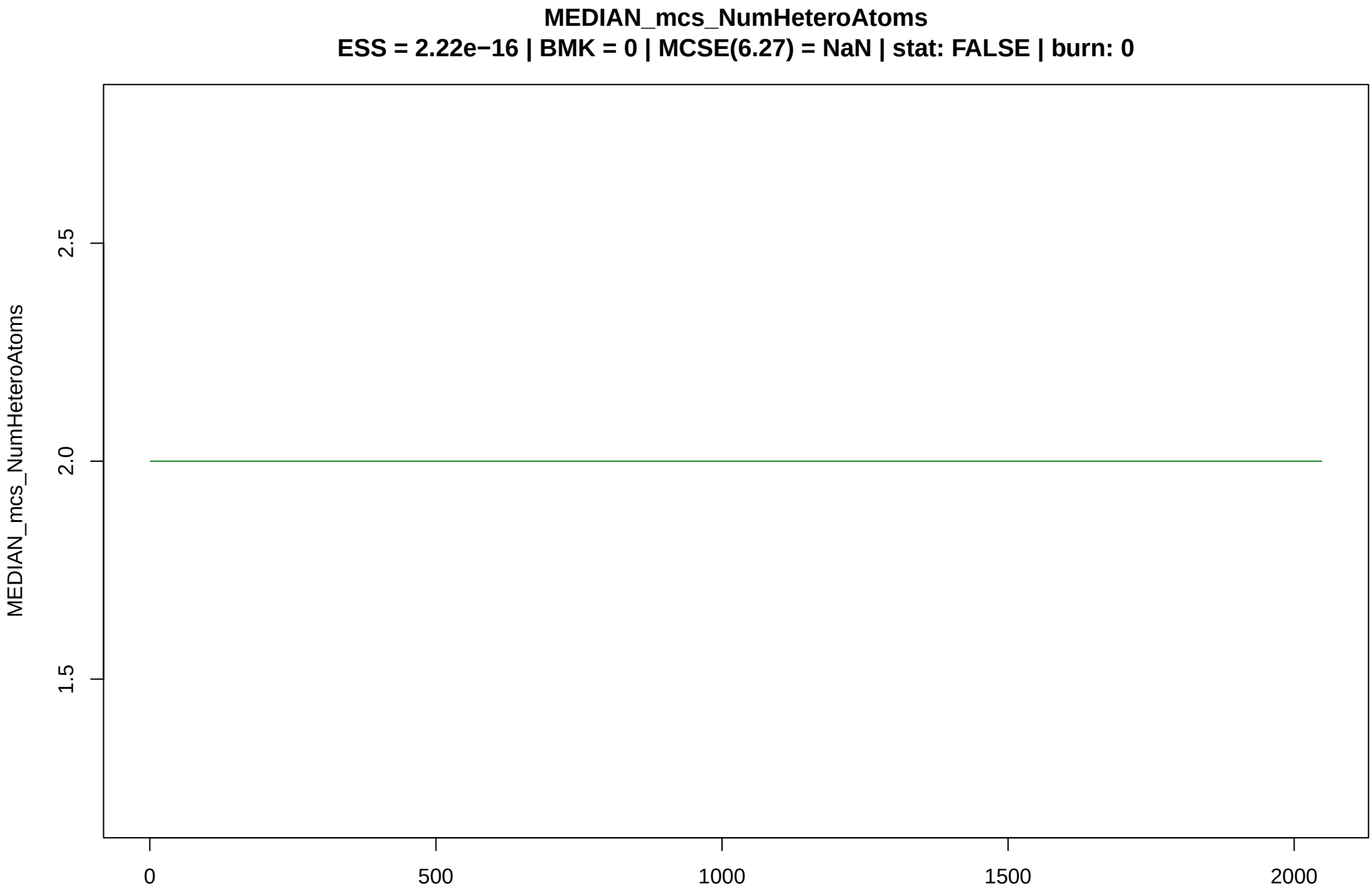

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0446 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 2040
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

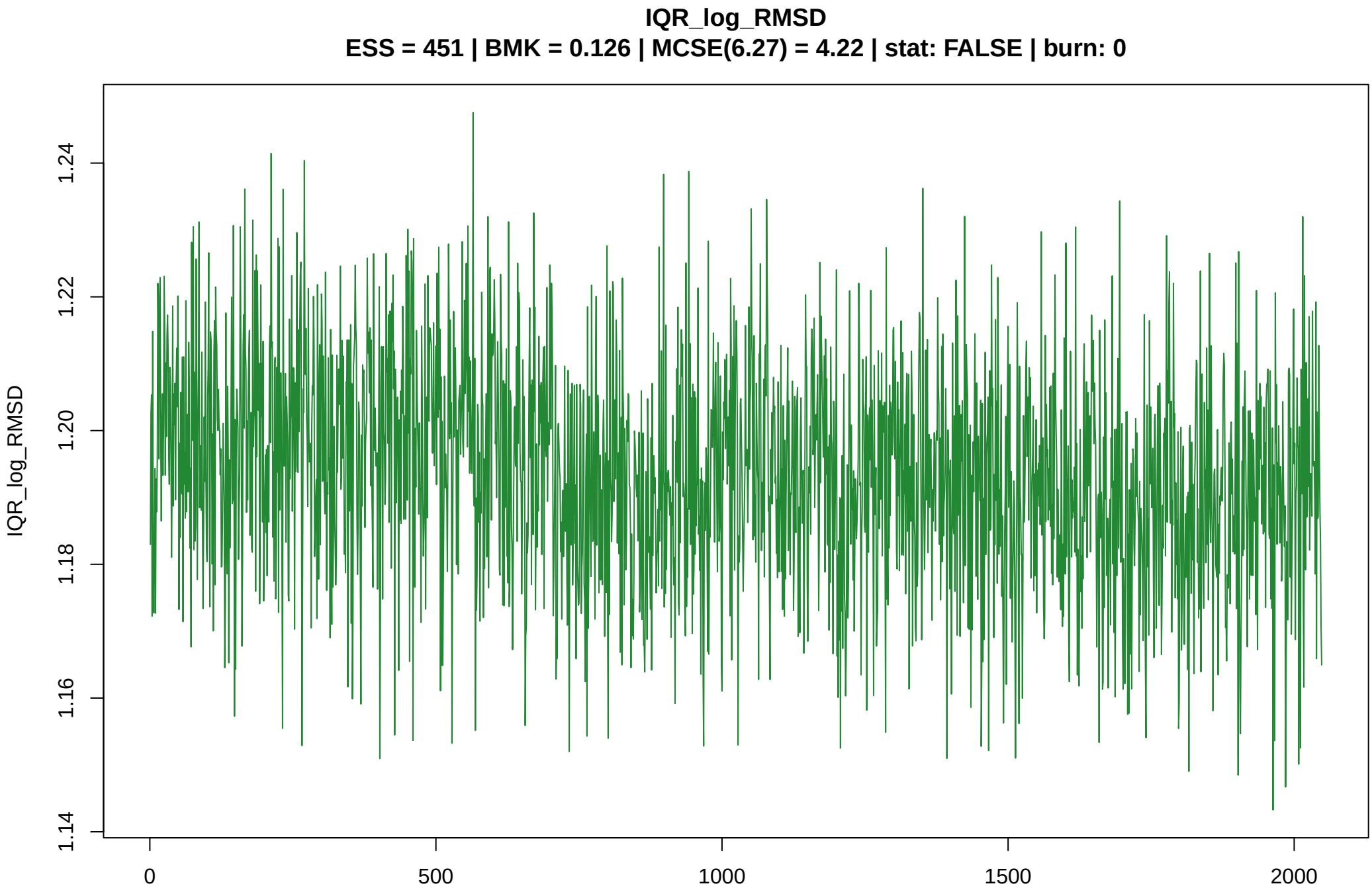

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

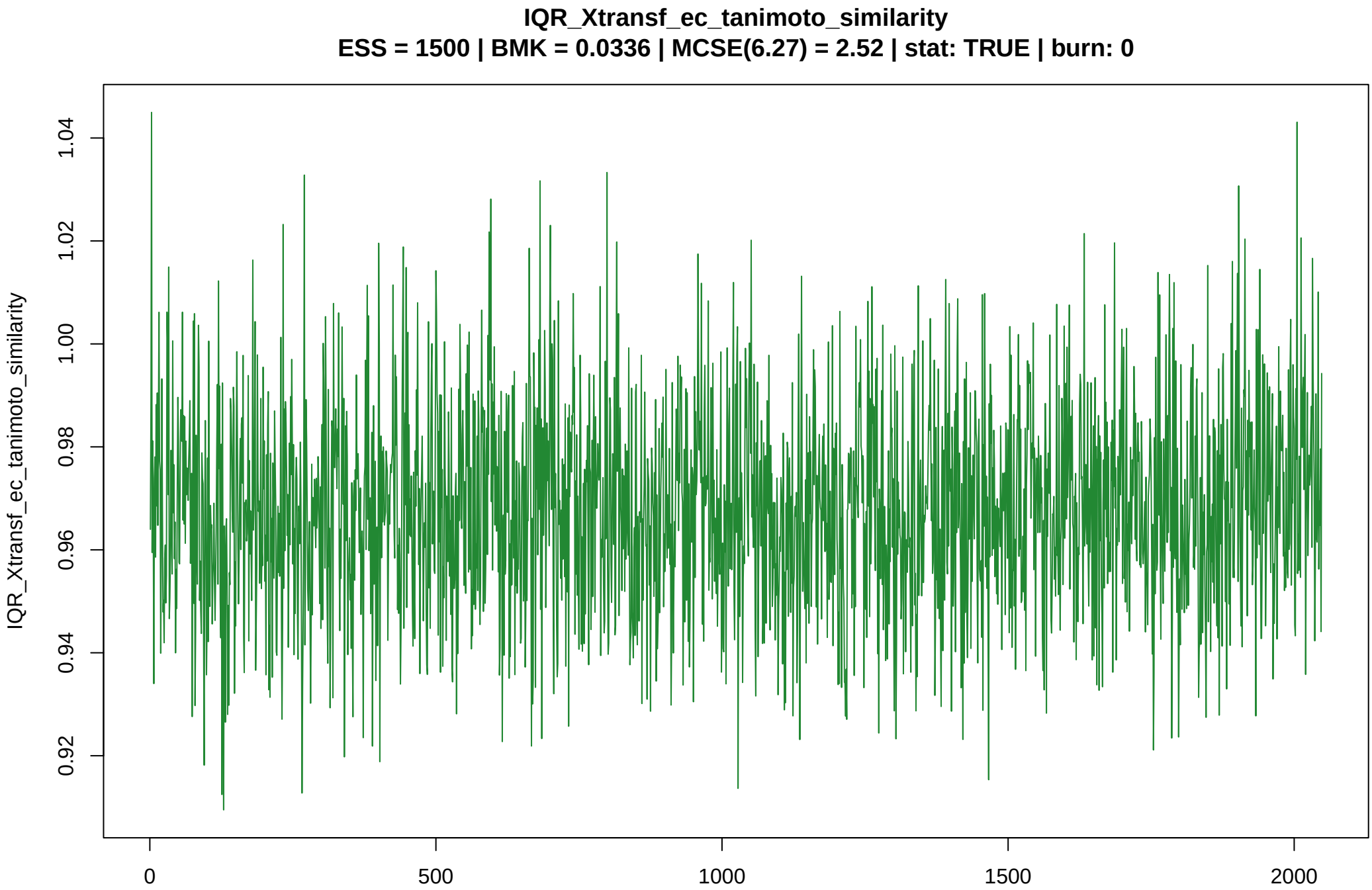

MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 1428
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

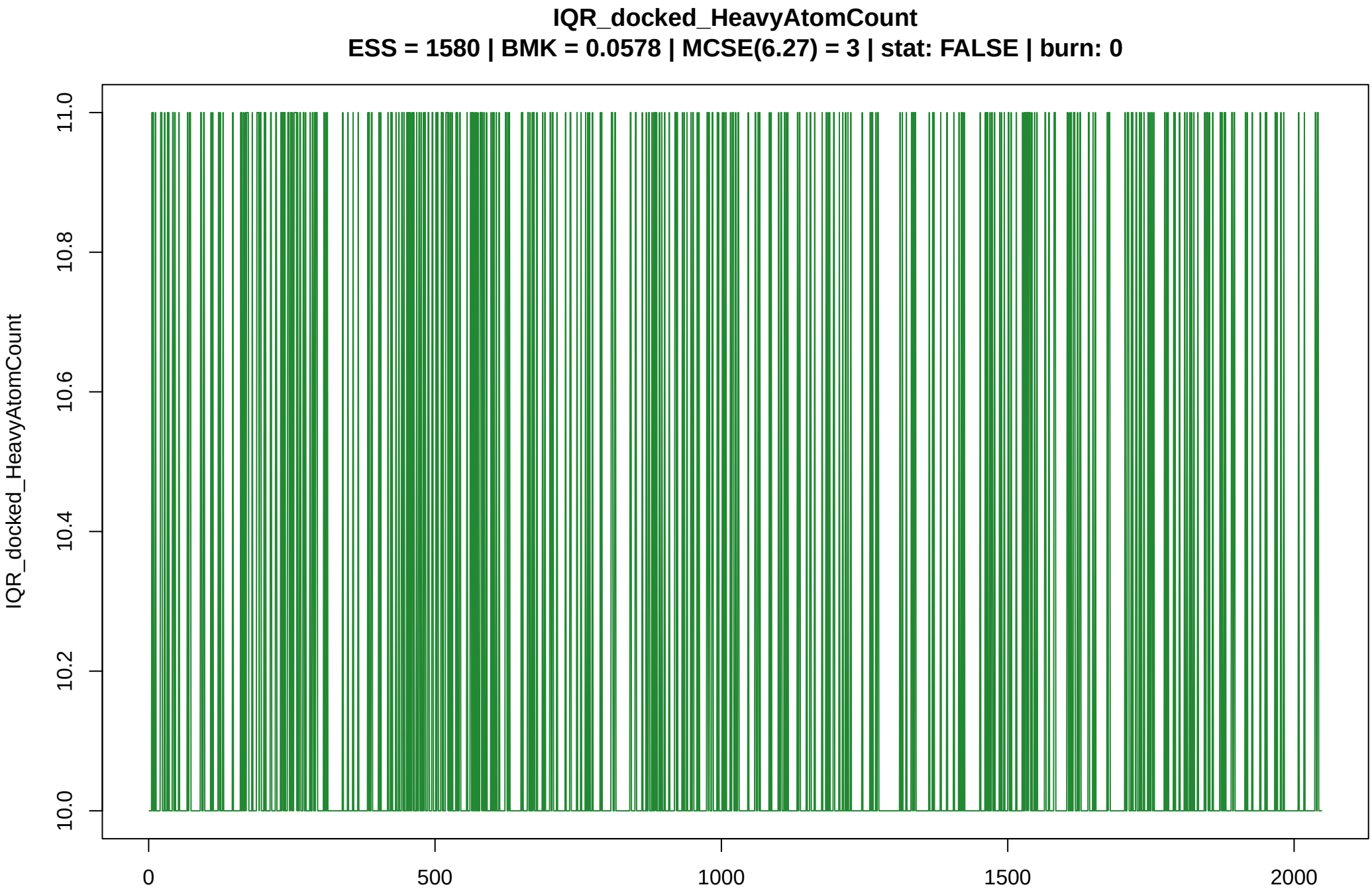

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

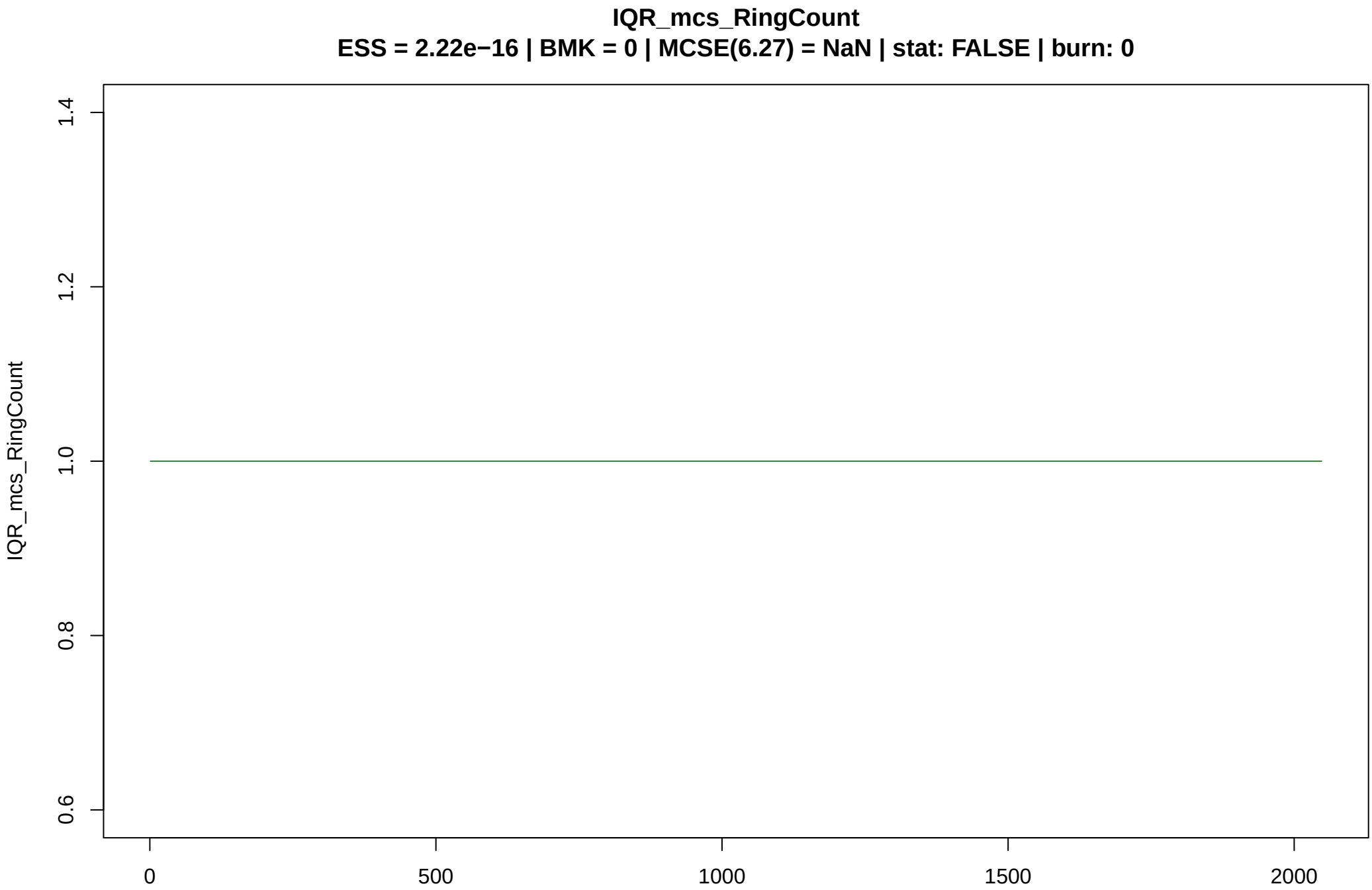

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

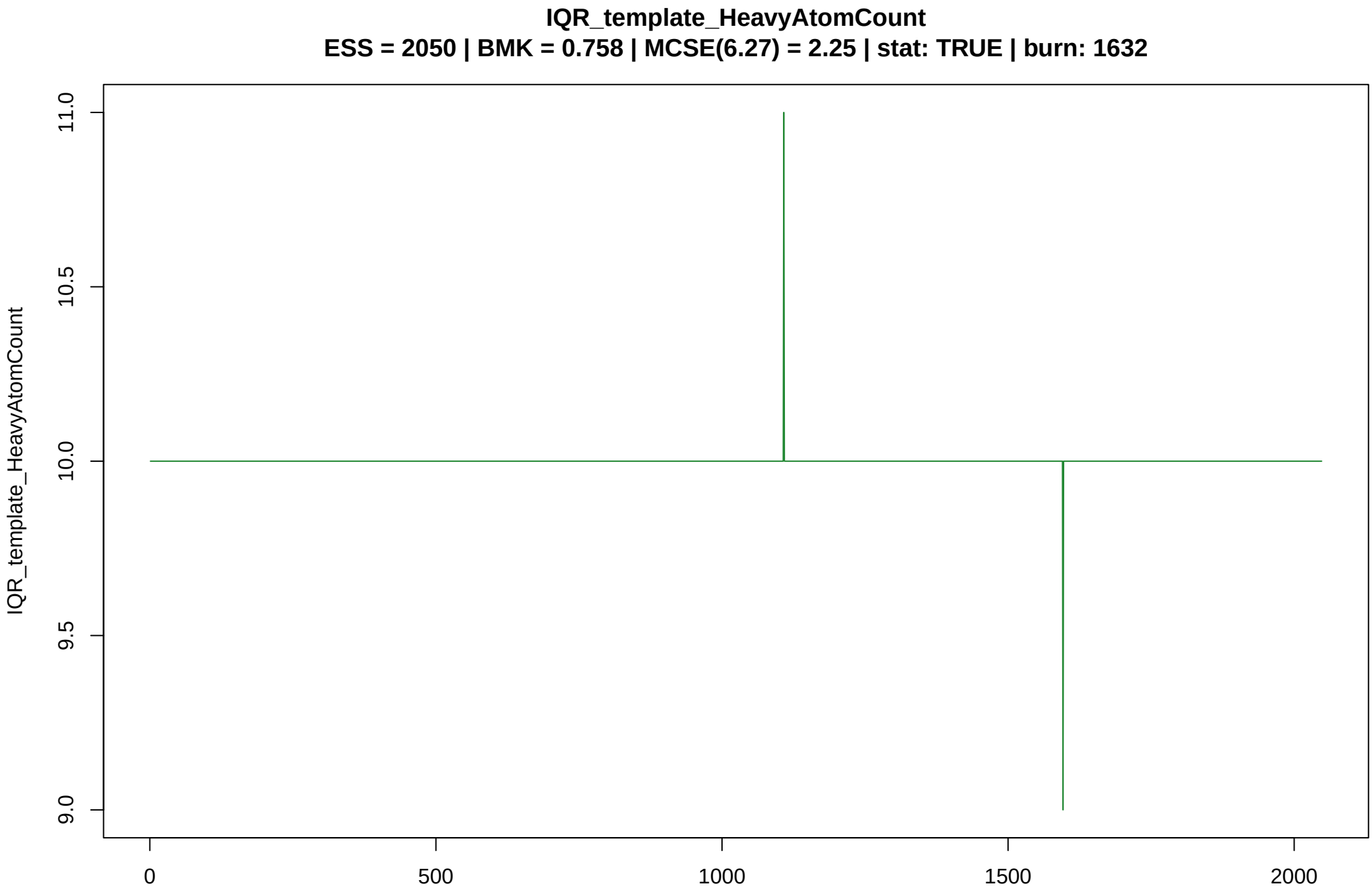

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

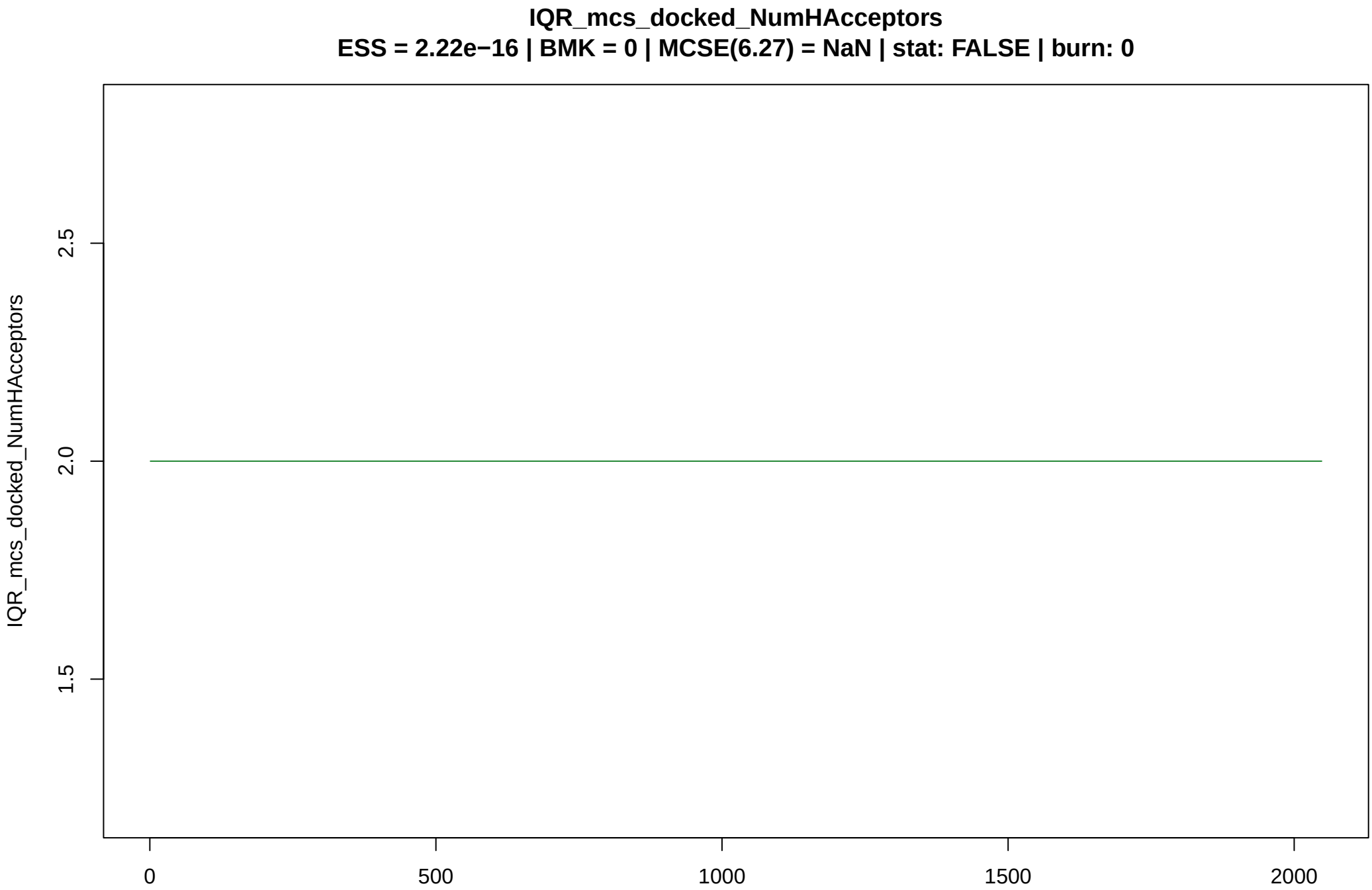

IQR_log_RMSD
ESS = 451 | BMK = 0.126 | MCSE(6.27) = 4.22 | stat: FALSE | burn: 0
IQR_log_RMSD
1.14
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

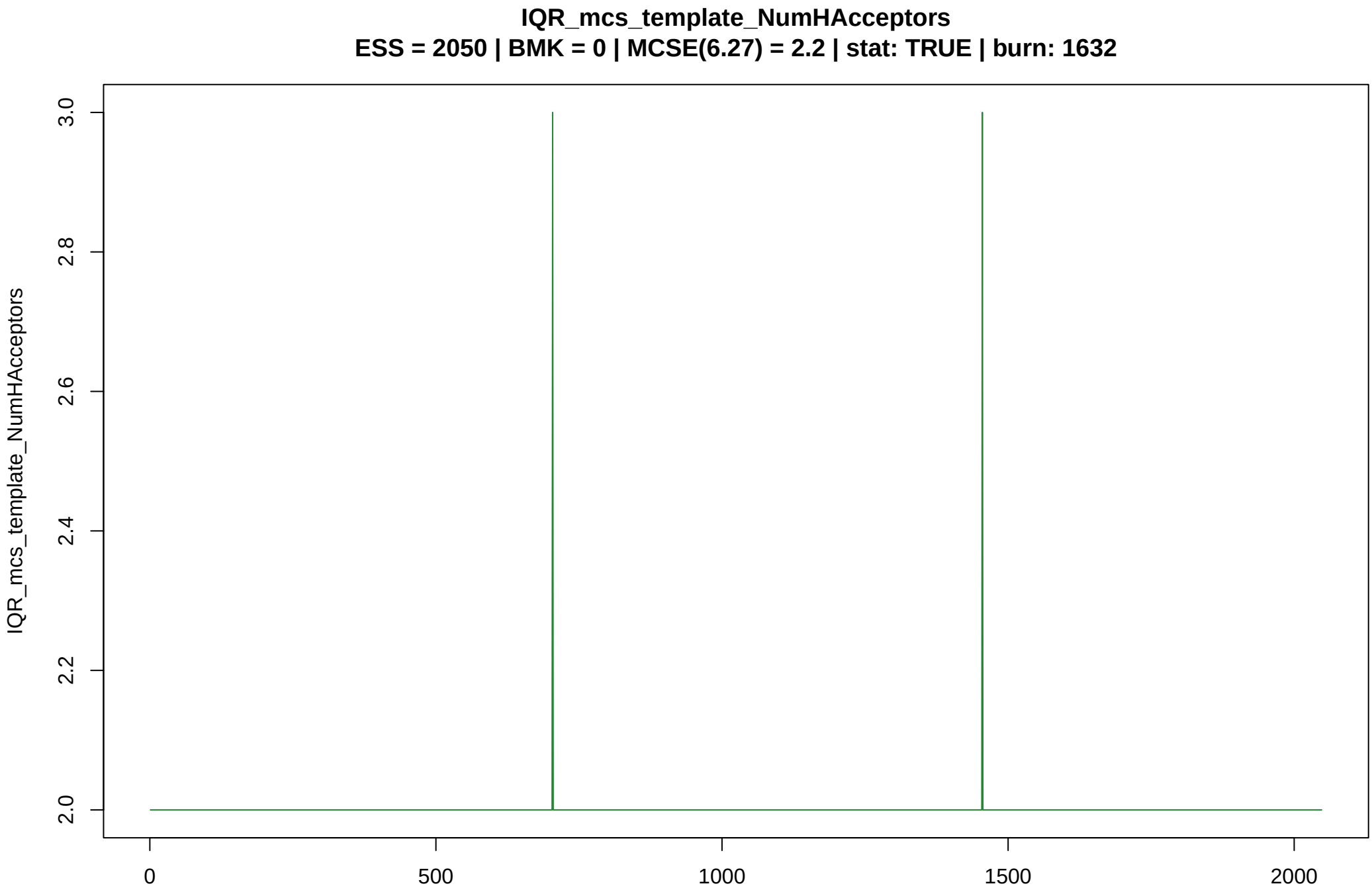

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1500 | BMK = 0.0336 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.92
0.94
0.96
0.98
1.00
1.02
1.04
0
500
1000
1500
2000

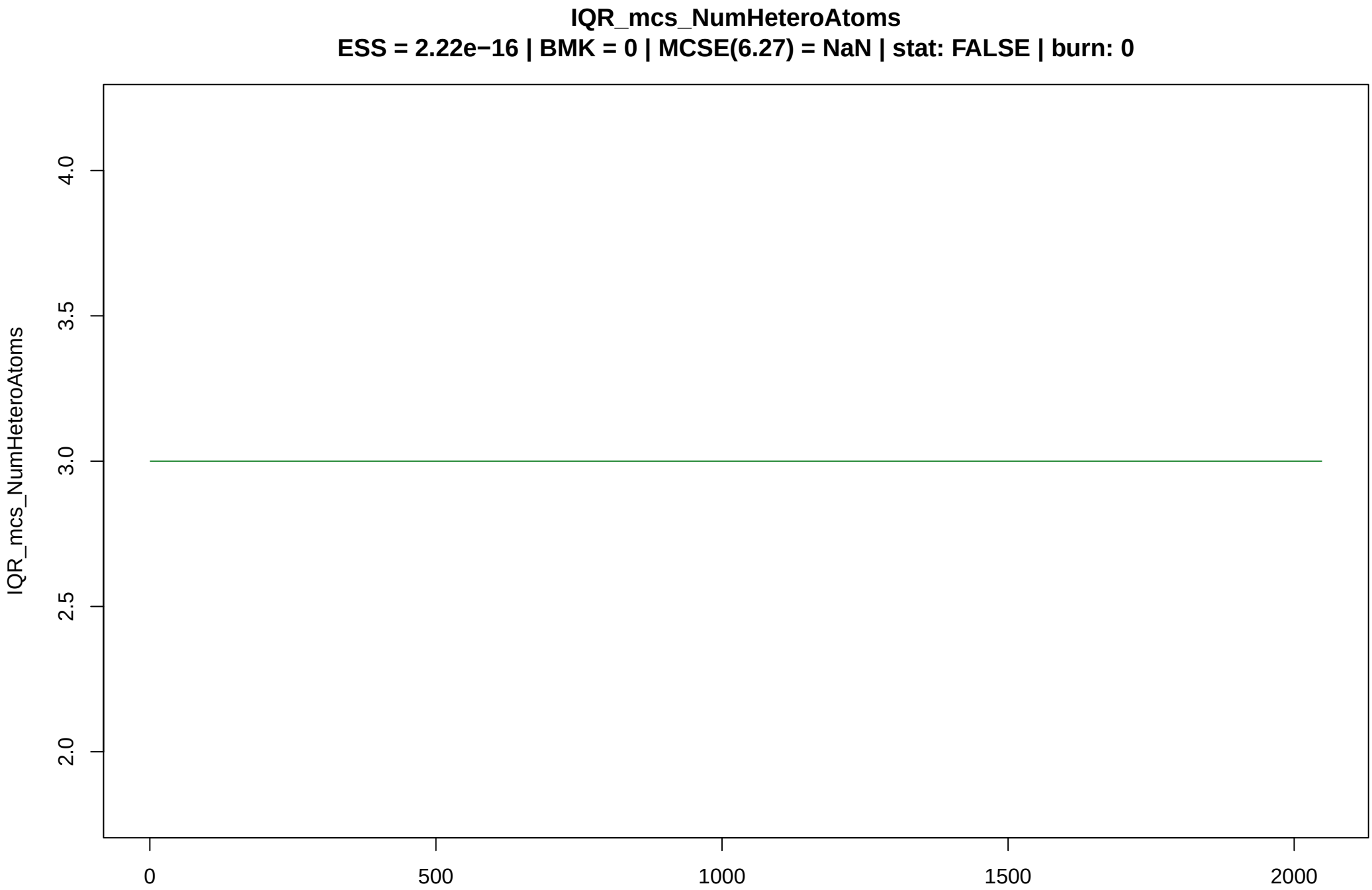

IQR_docked_HeavyAtomCount
ESS = 1580 | BMK = 0.0578 | MCSE(6.27) = 3 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
10.0
10.2
10.4
10.6
10.8
11.0
0
500
1000
1500
2000

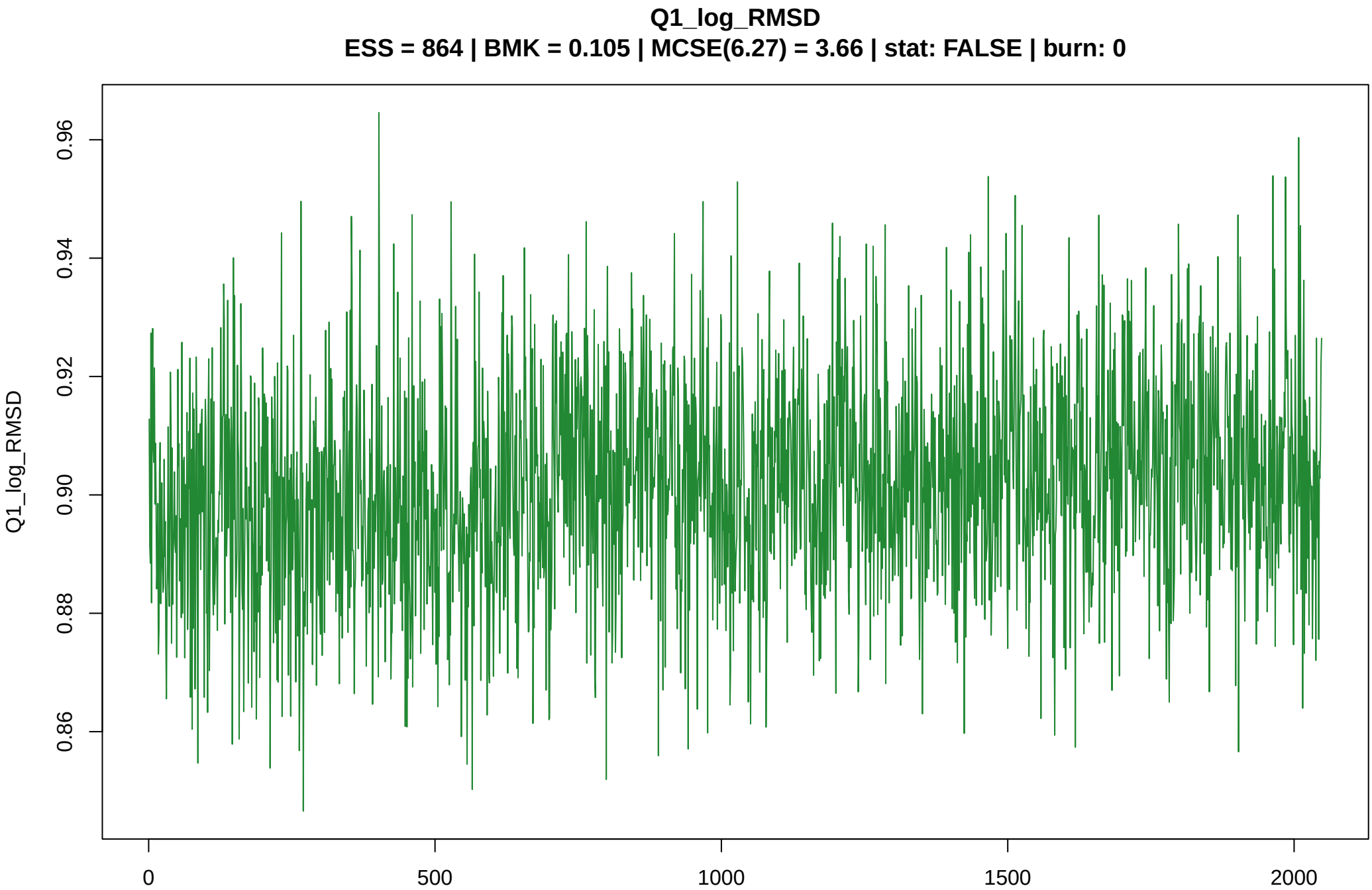

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

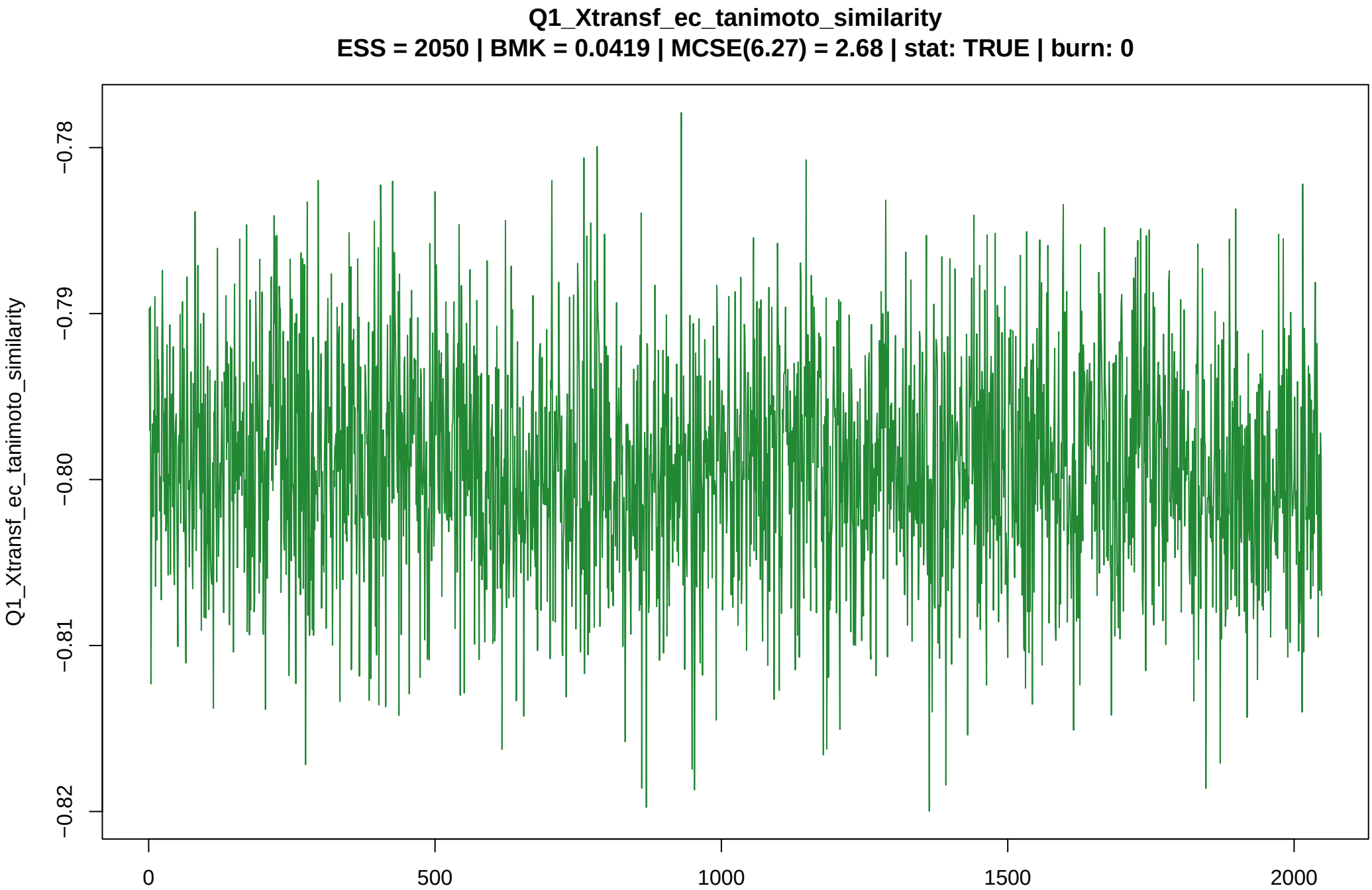

IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.758 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 1632
IQR_template_HeavyAtomCount
11.0
10.5
10.0
9.5
9.0
0
500
1000
1500
2000

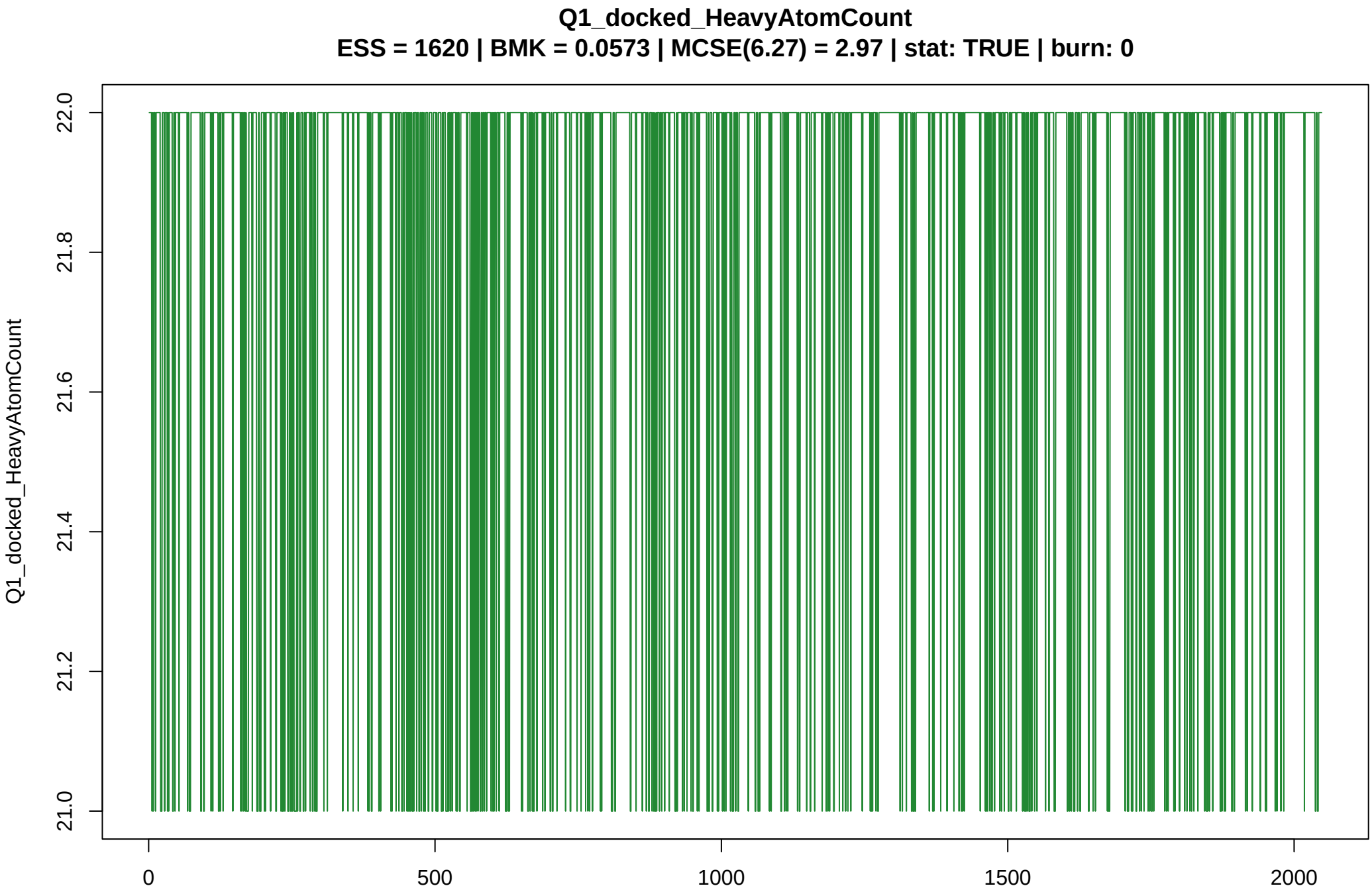

IQR_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_docked_NumHAcceptors
2.5
2.0
1.5
0
500
1000
1500
2000

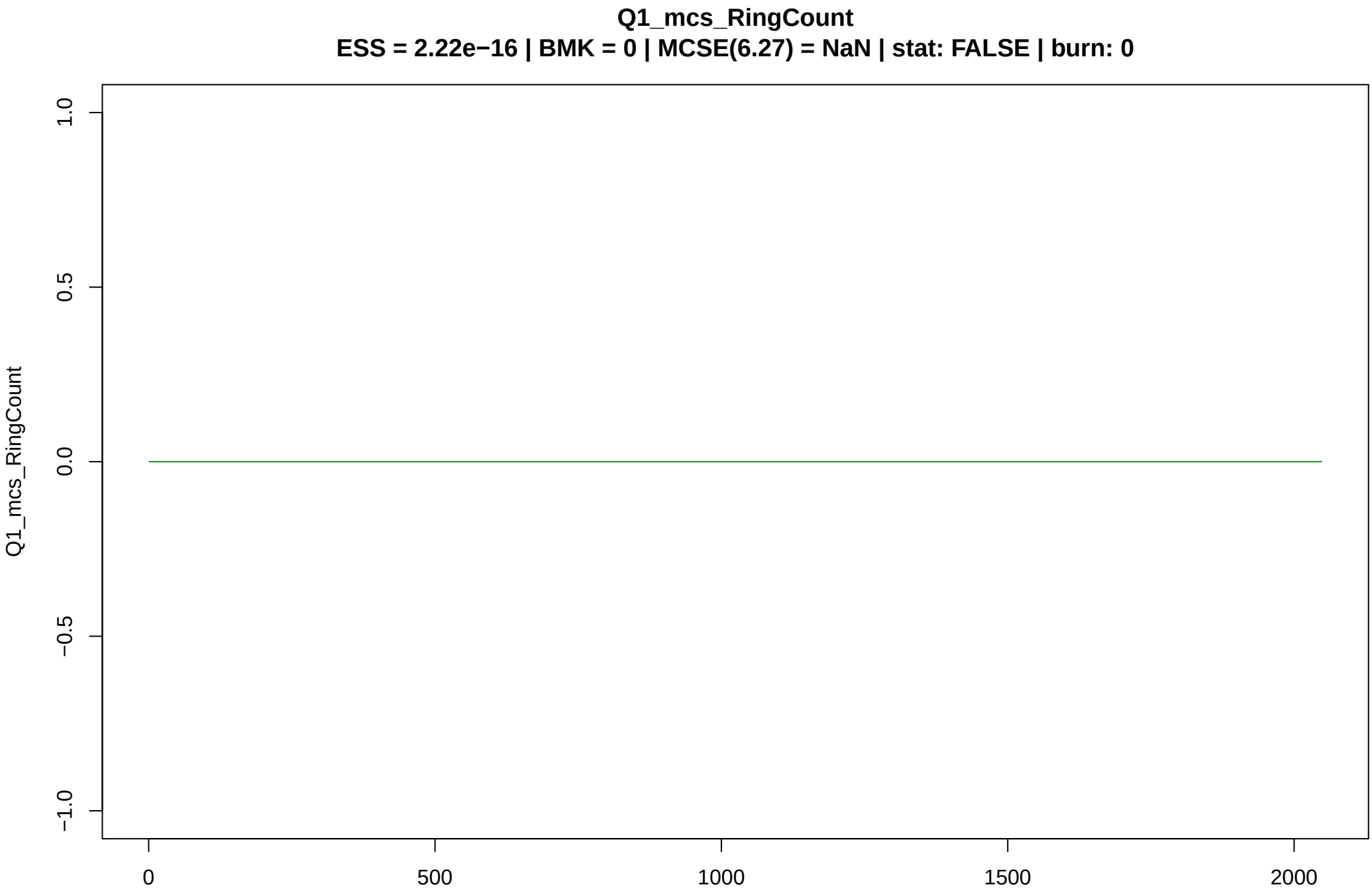

IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632
IQR_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

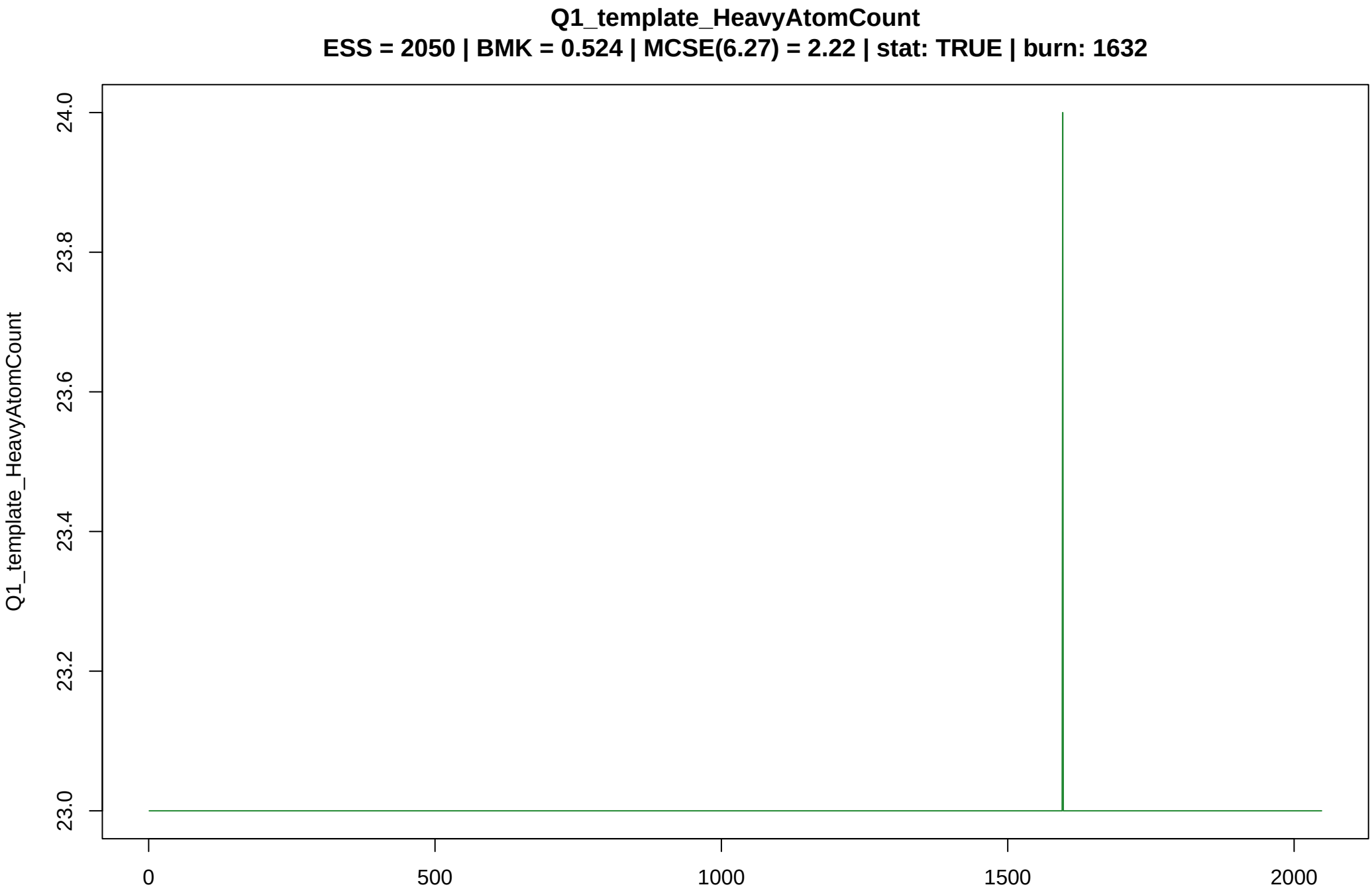

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

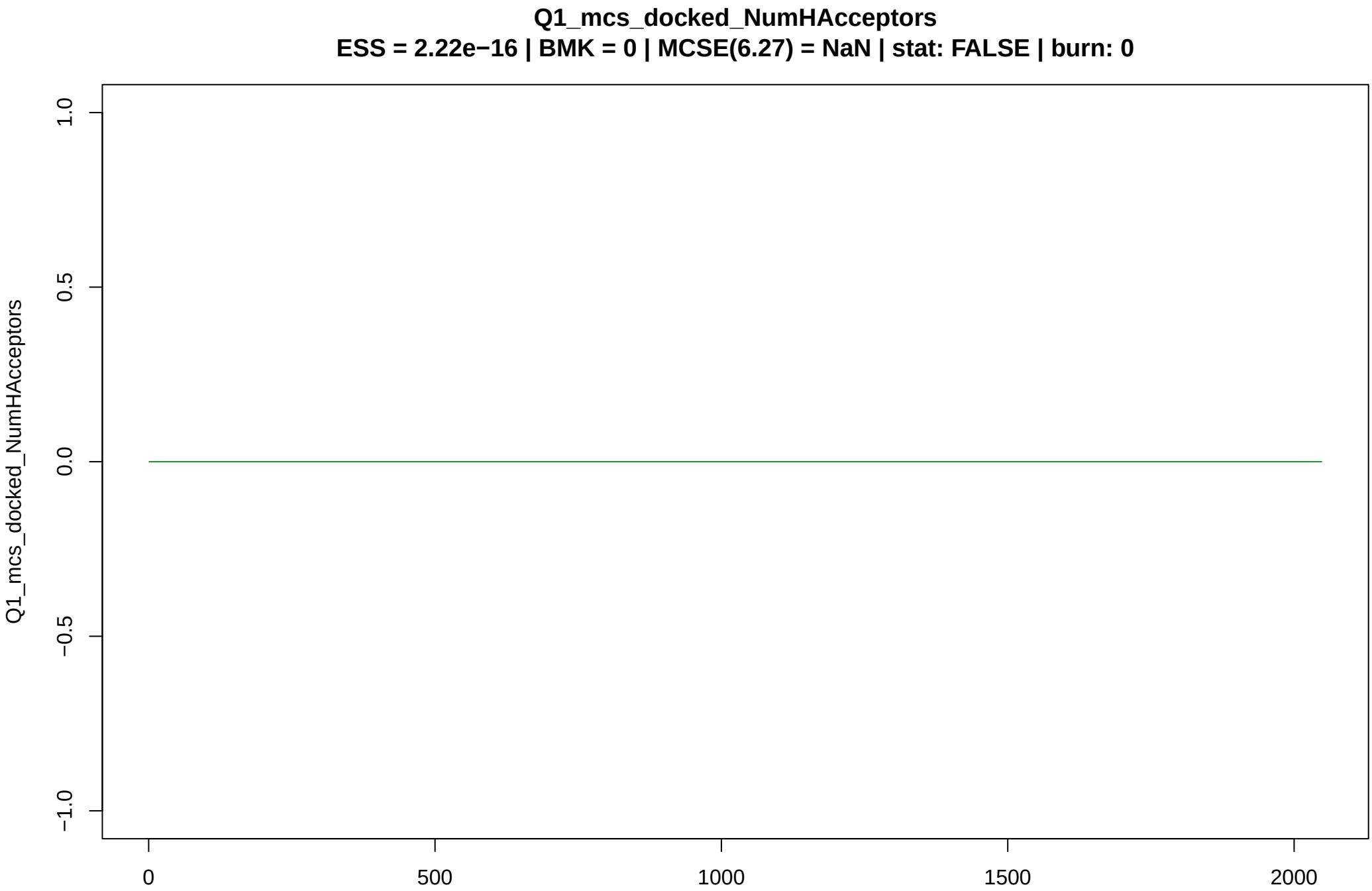

Q1_log_RMSD
ESS = 864 | BMK = 0.105 | MCSE(6.27) = 3.66 | stat: FALSE | burn: 0
Q1_log_RMSD
0.86
0.88
0.90
0.92
0.94
0.96
0
500
1000
1500
2000

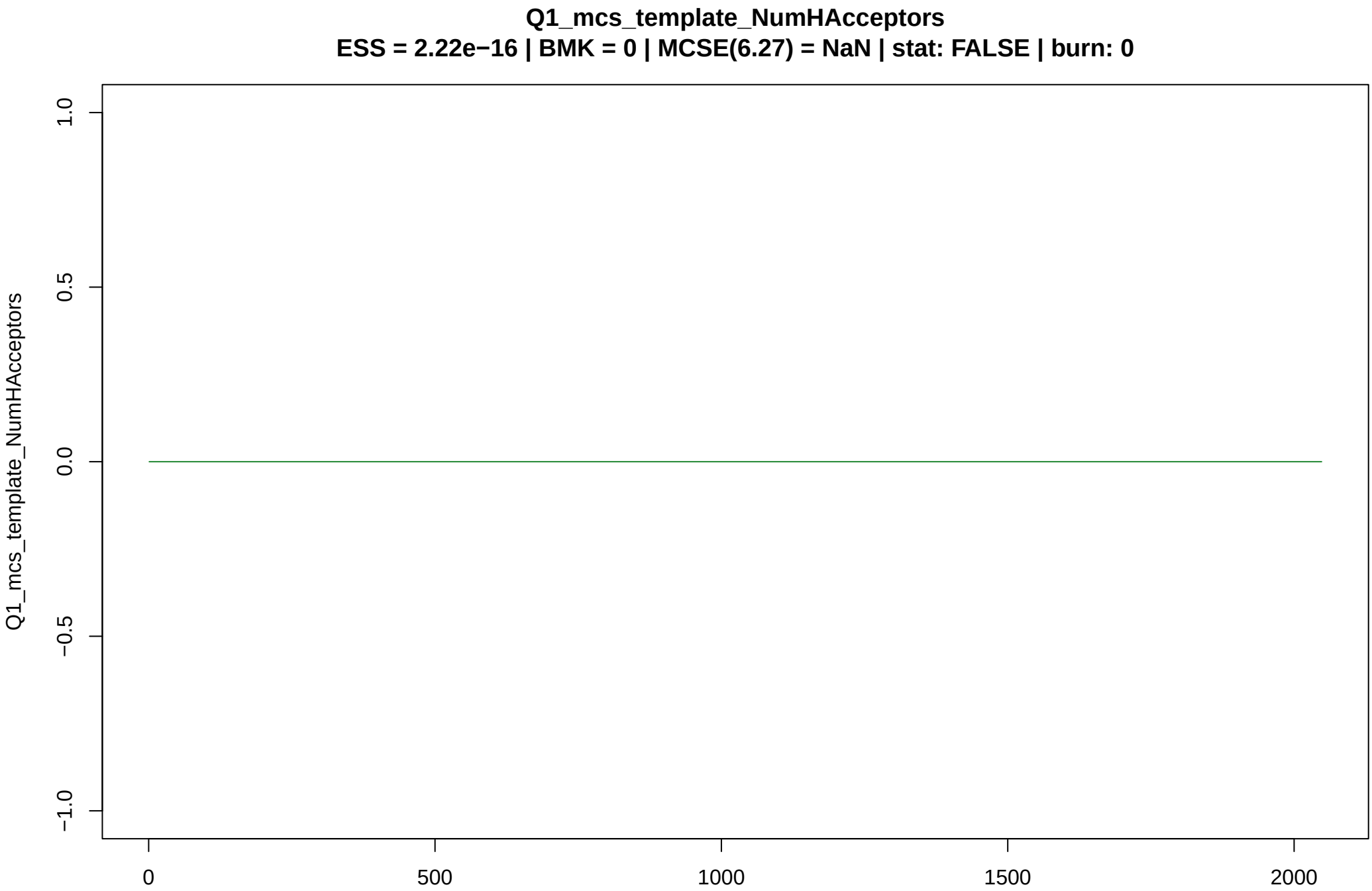

Q1_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

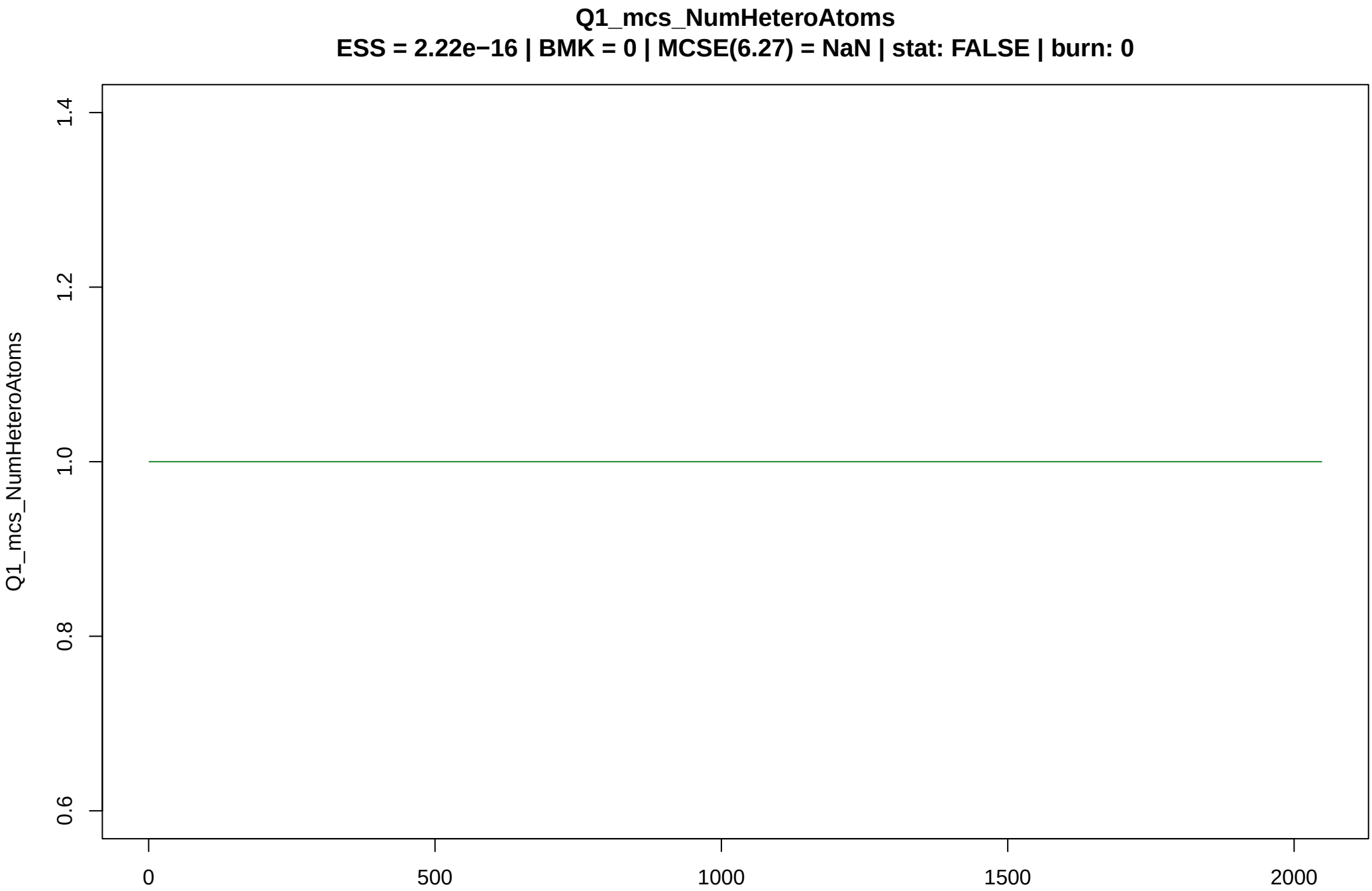

Q1_docked_HeavyAtomCount
ESS = 1620 | BMK = 0.0573 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

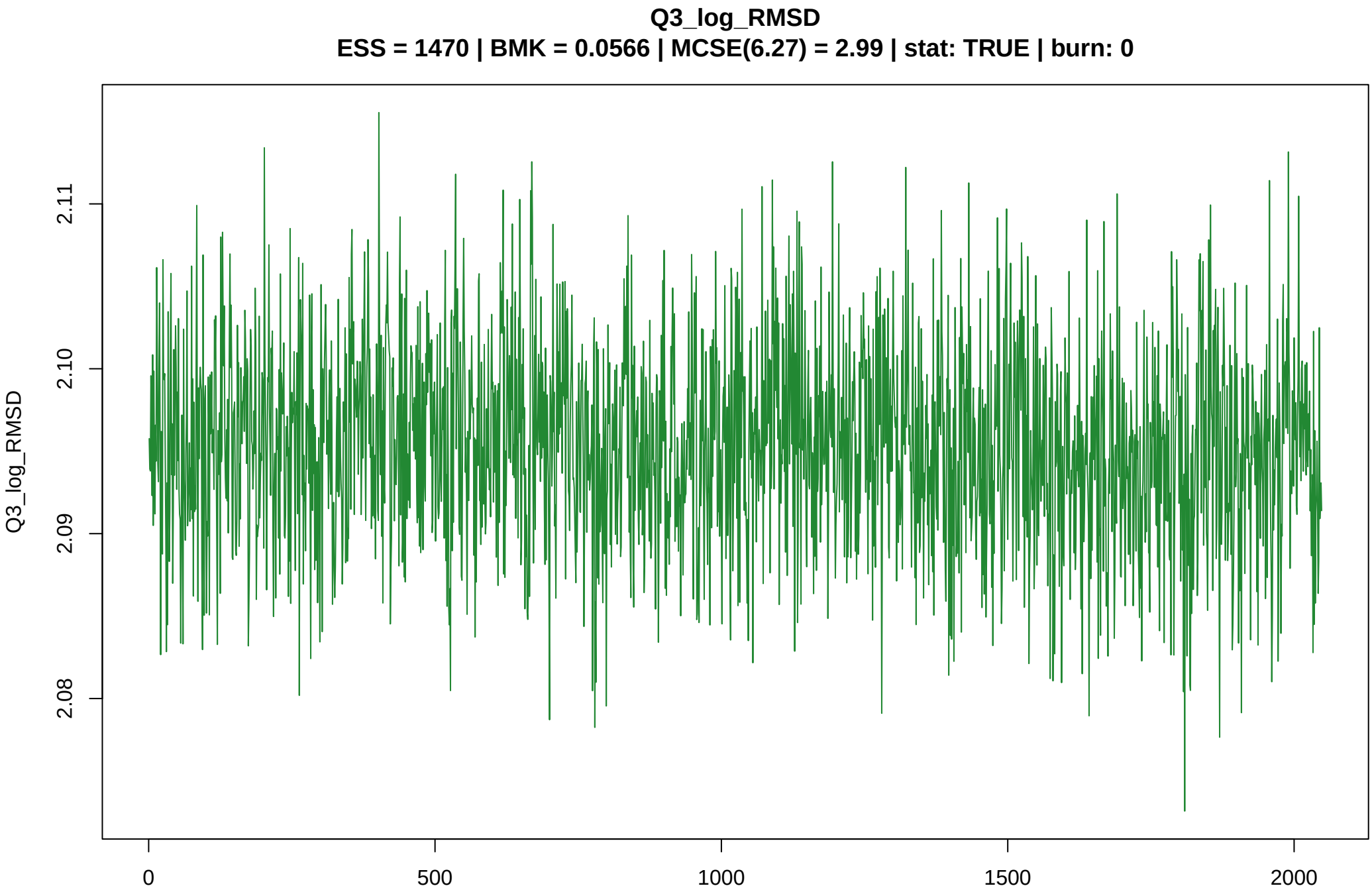

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

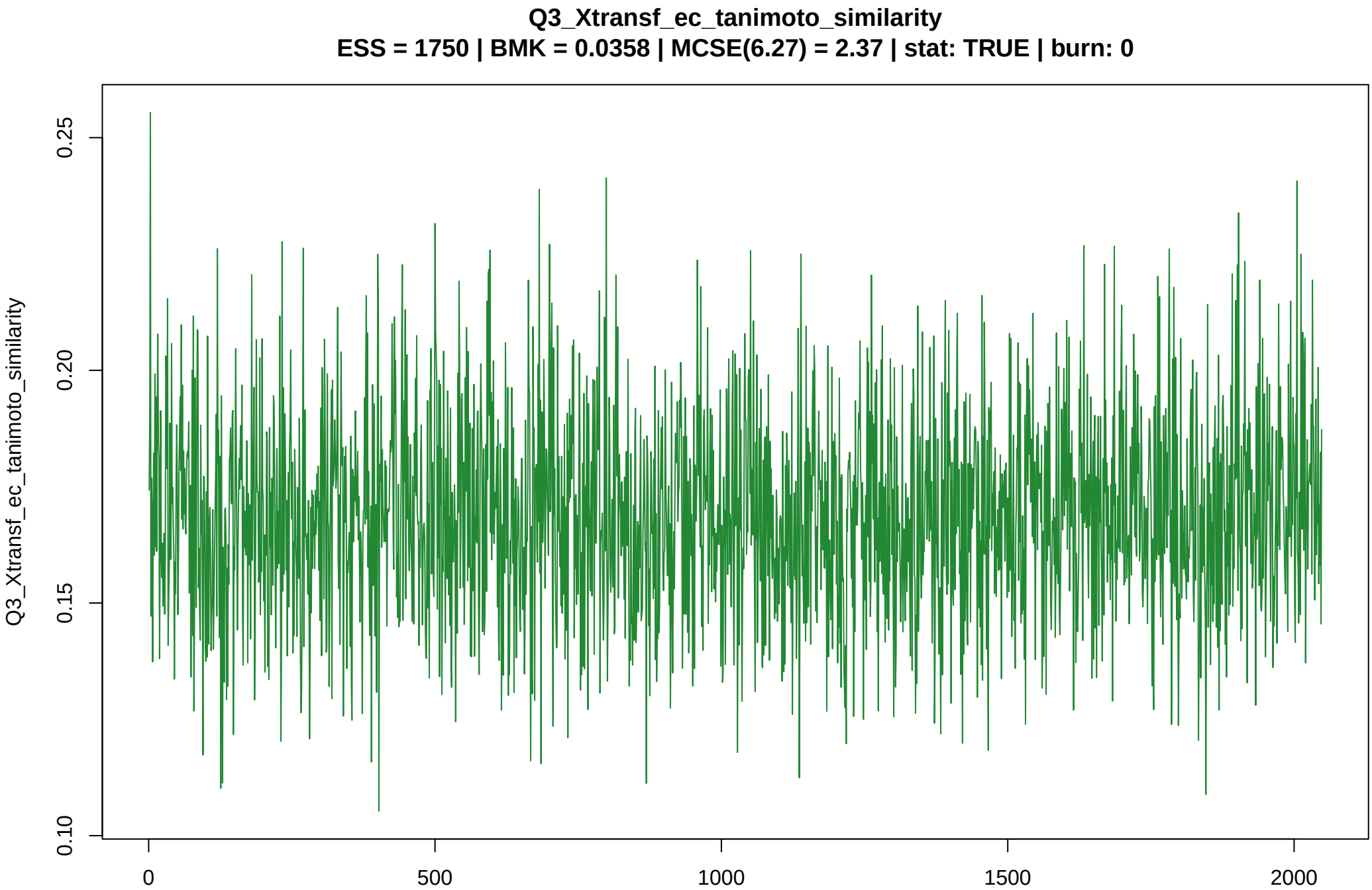

Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.524 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1632
Q1_template_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

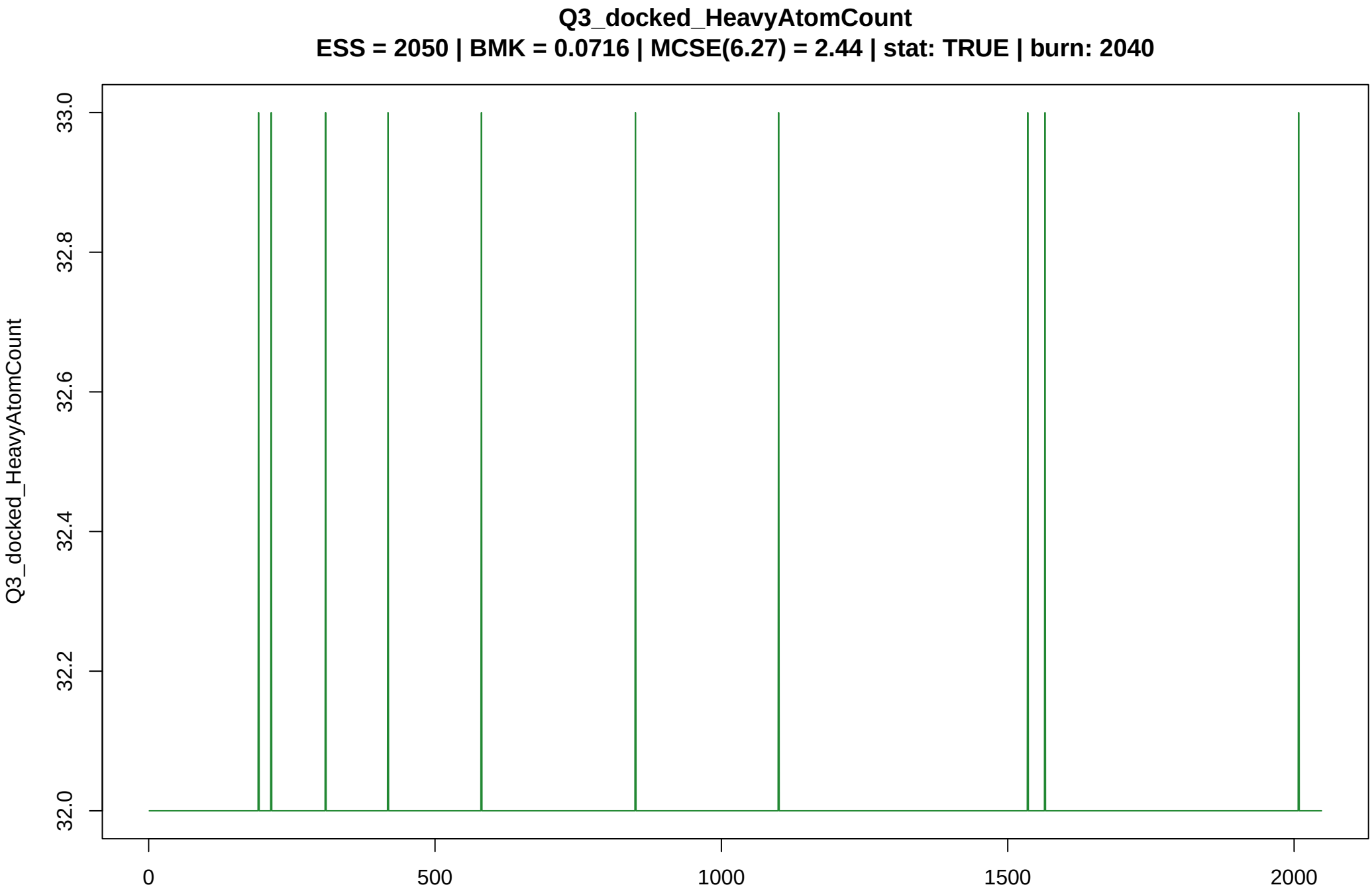

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

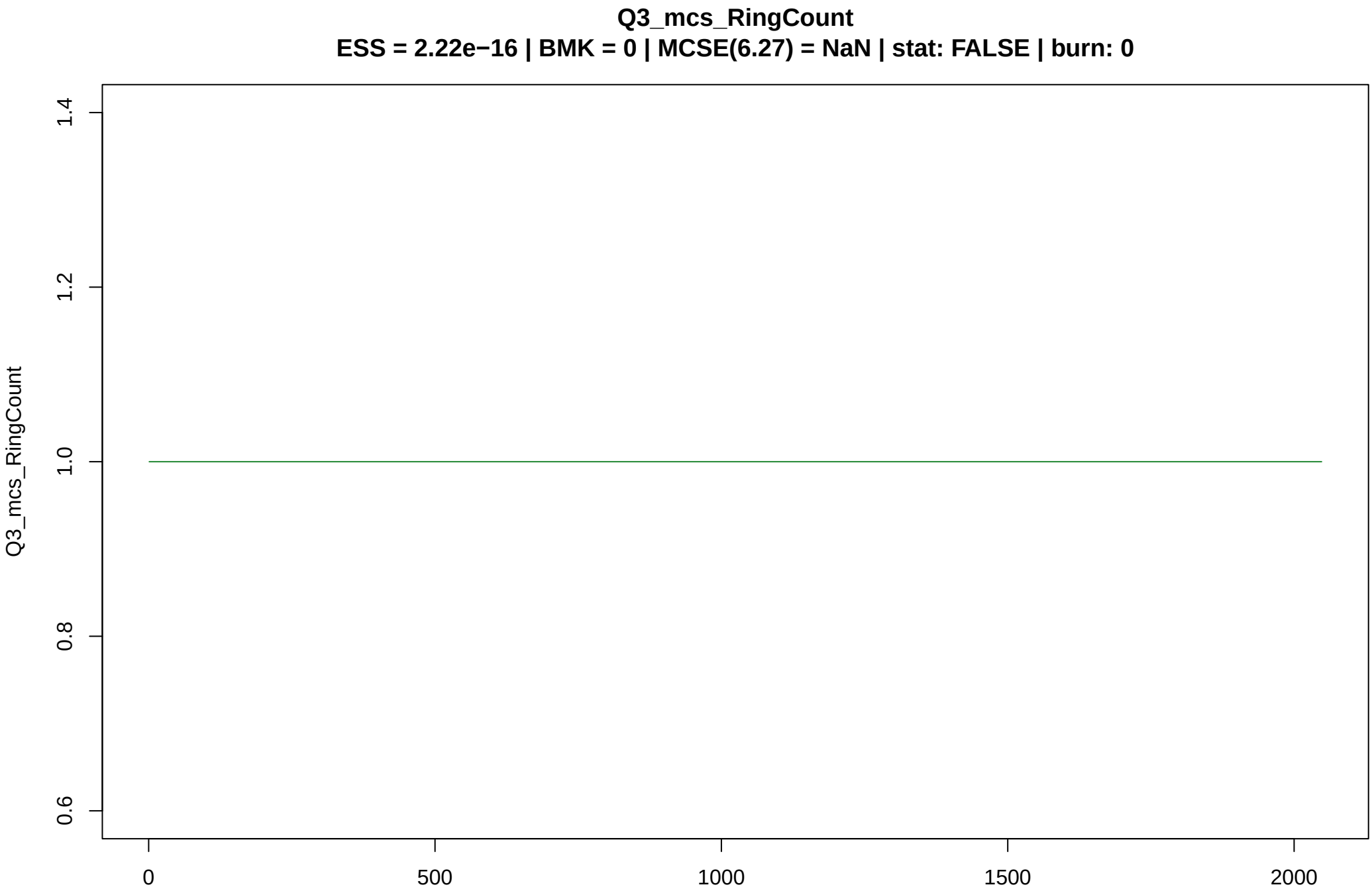

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

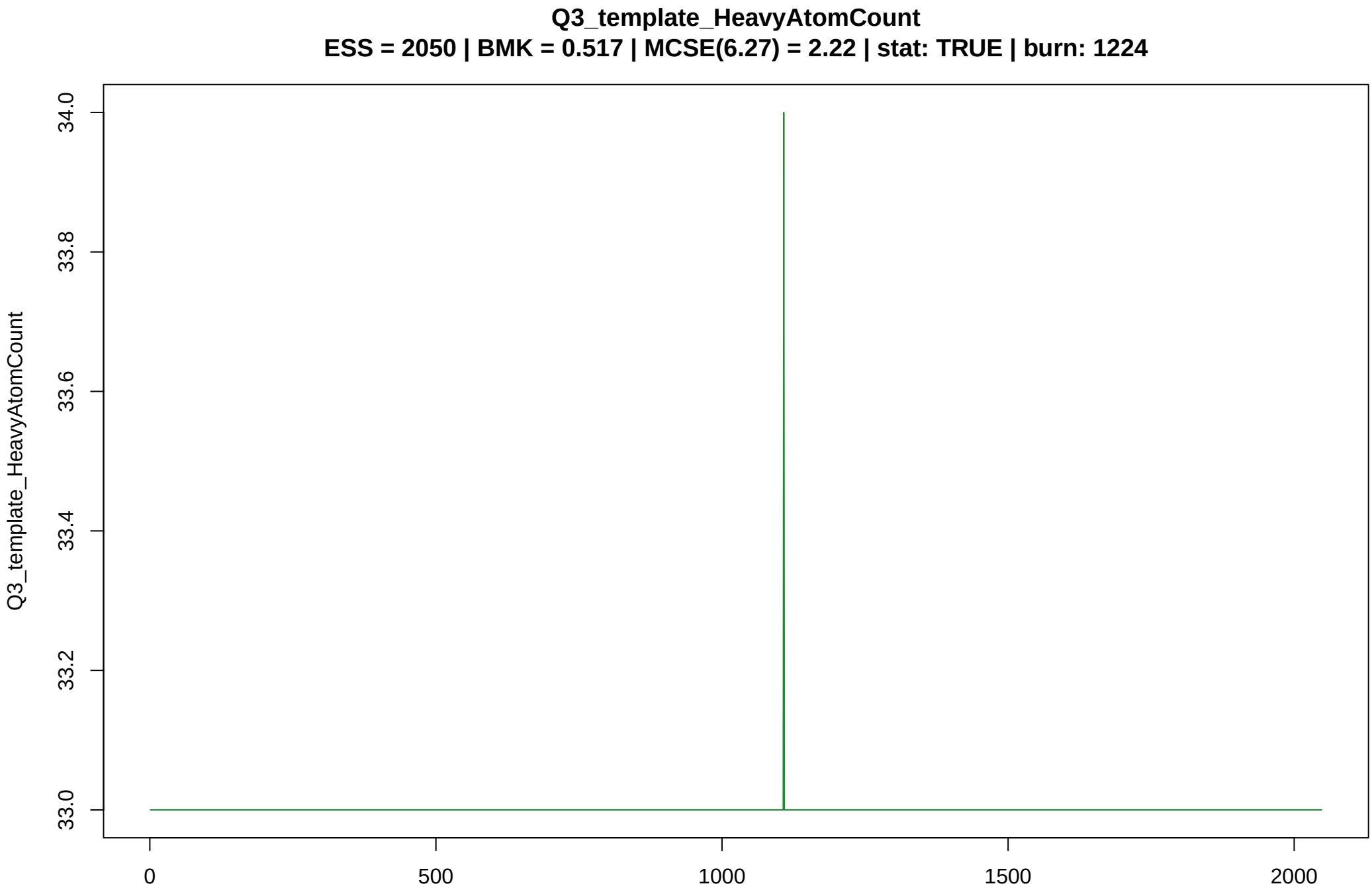

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

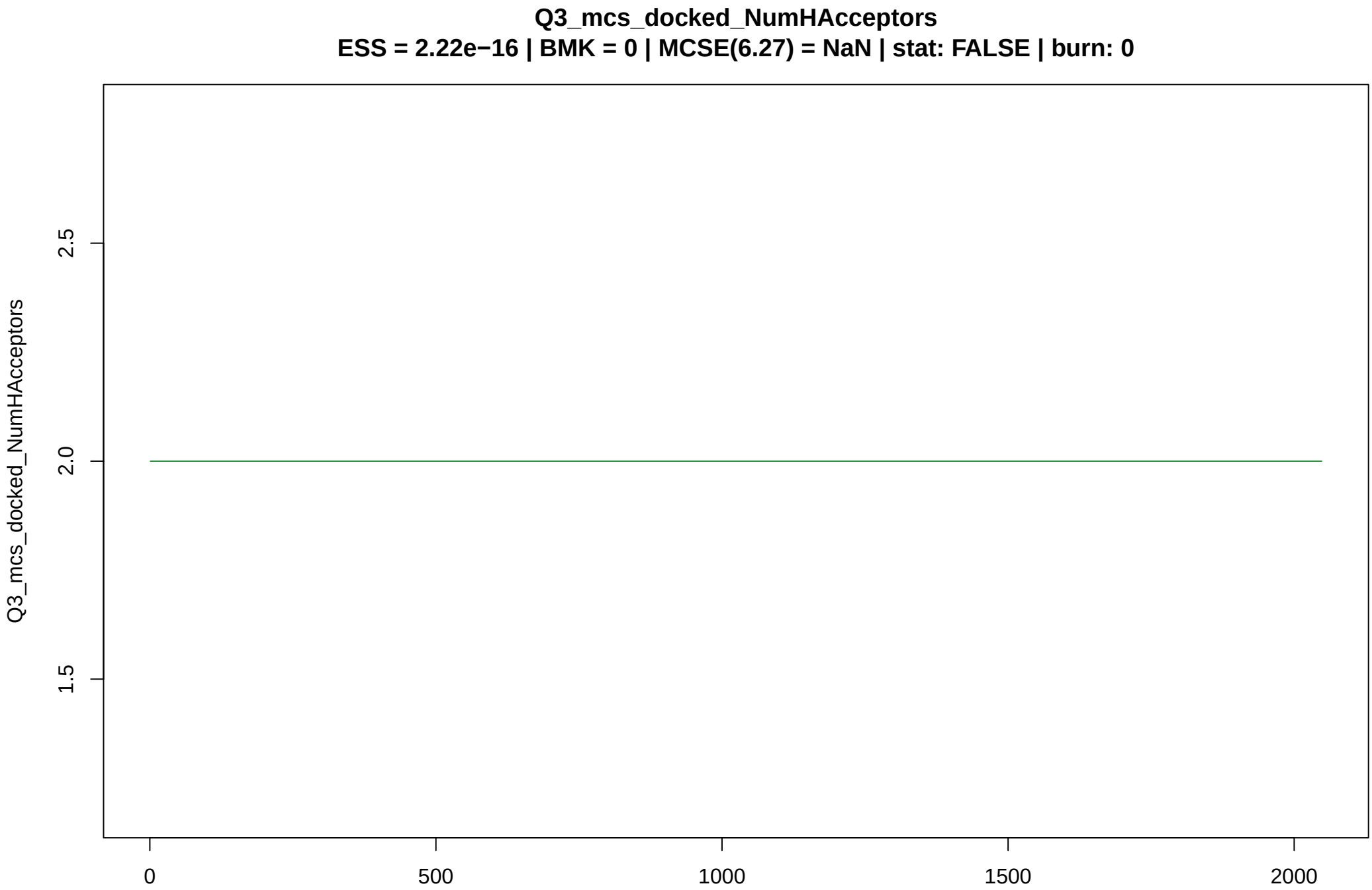

Q3_log_RMSD
ESS = 1470 | BMK = 0.0566 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

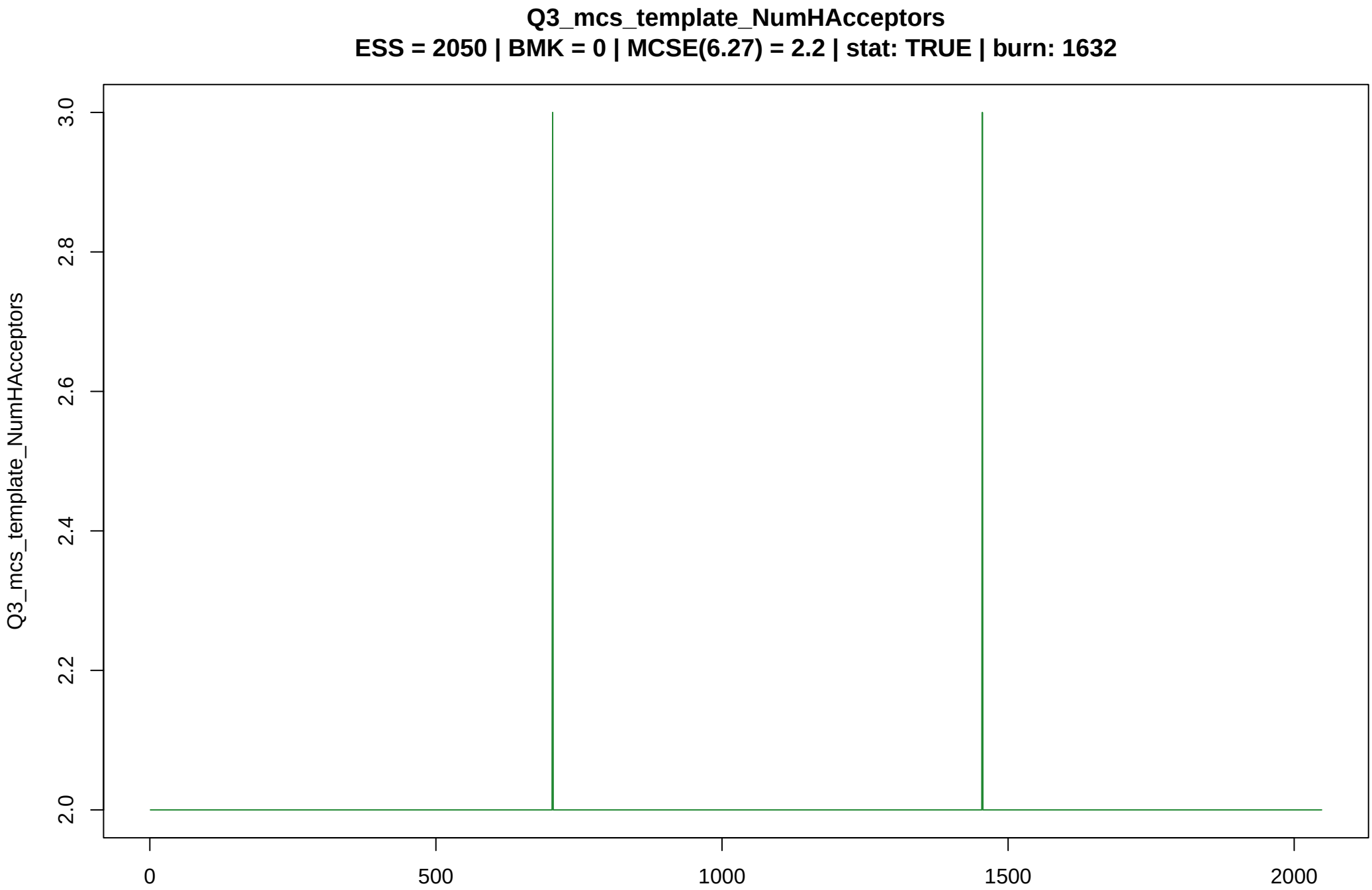

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1750 | BMK = 0.0358 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.10
0.15
0.20
0.25
0
500
1000
1500
2000

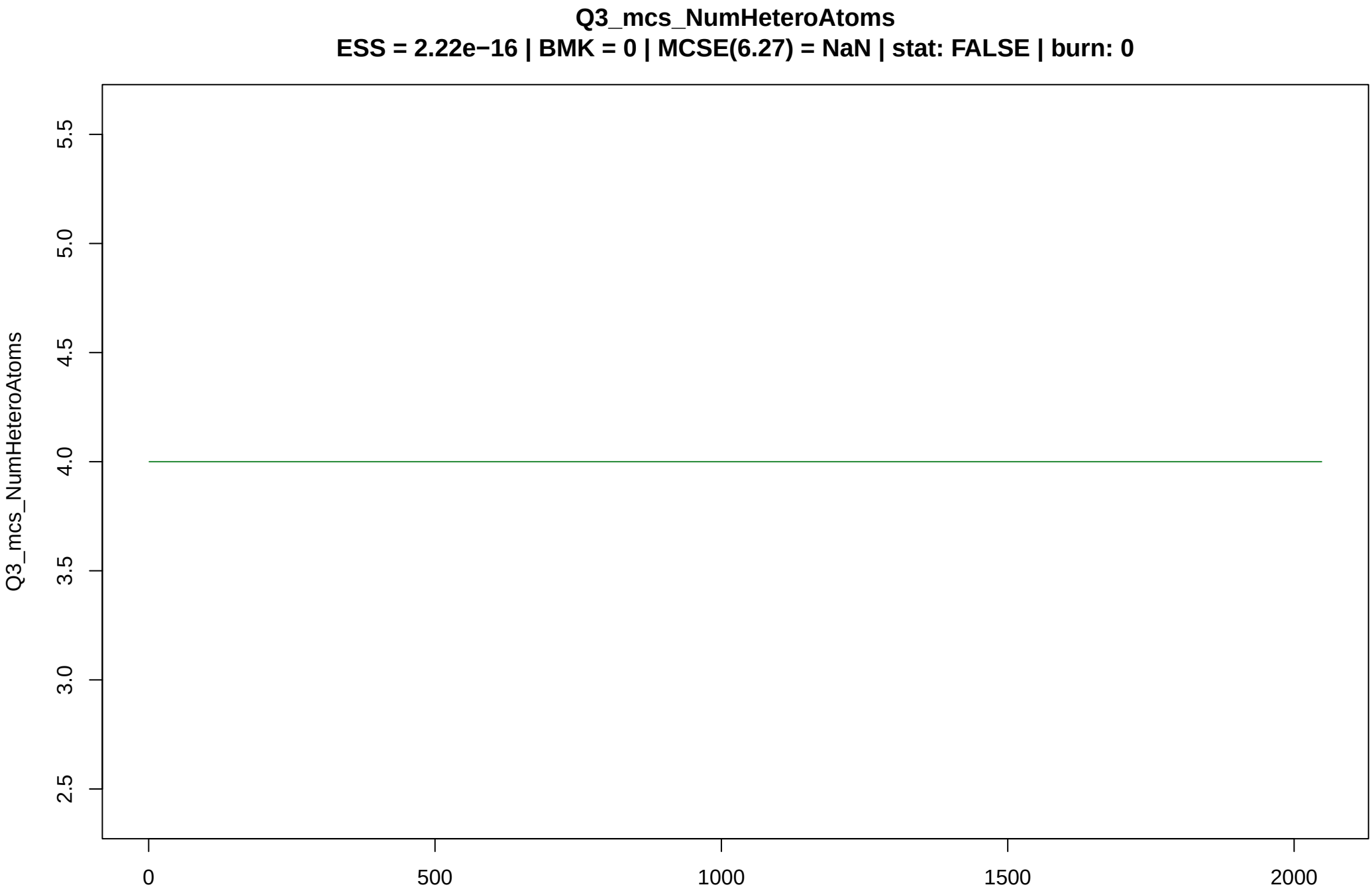

Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0716 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 2040
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

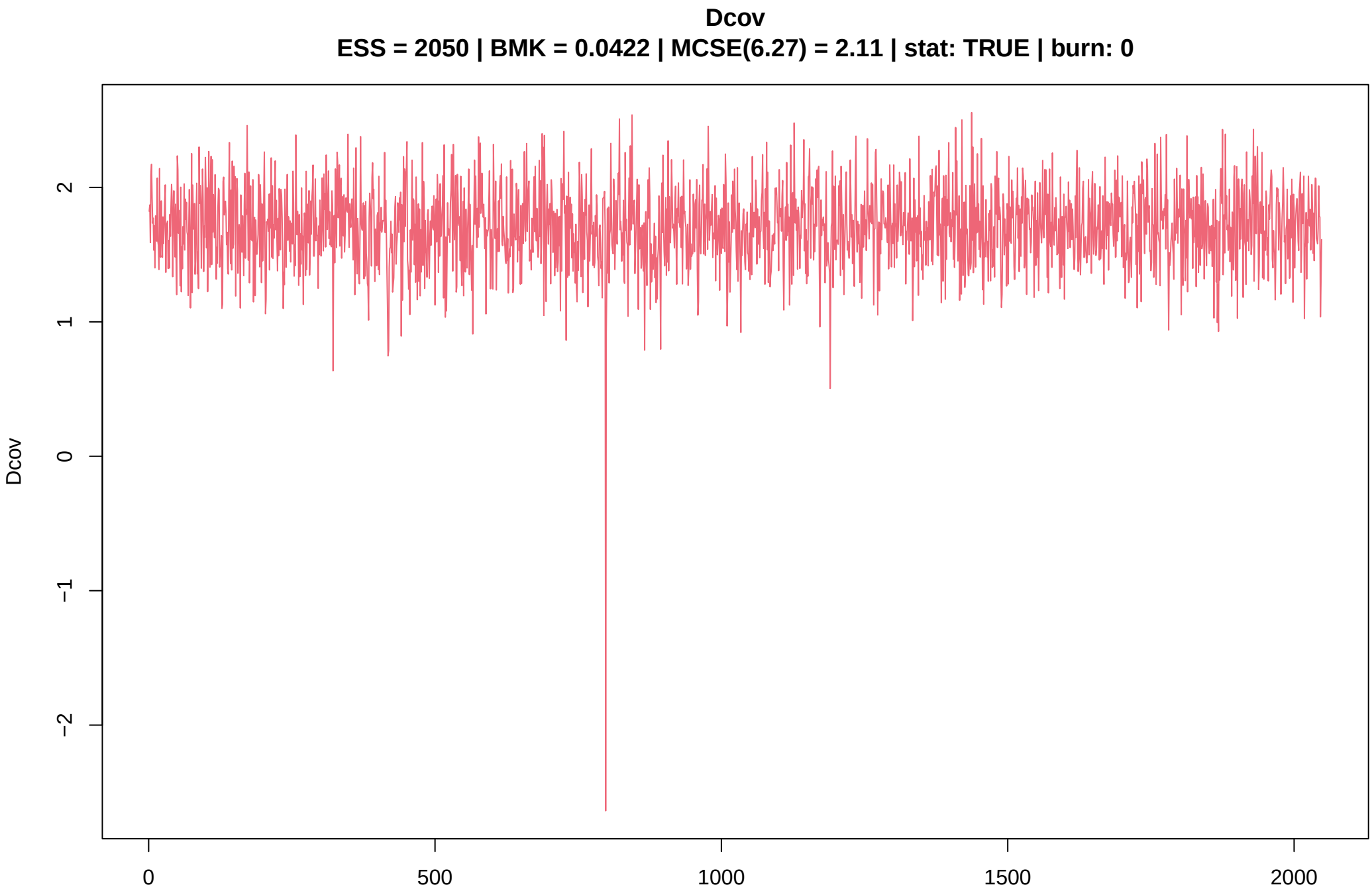

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

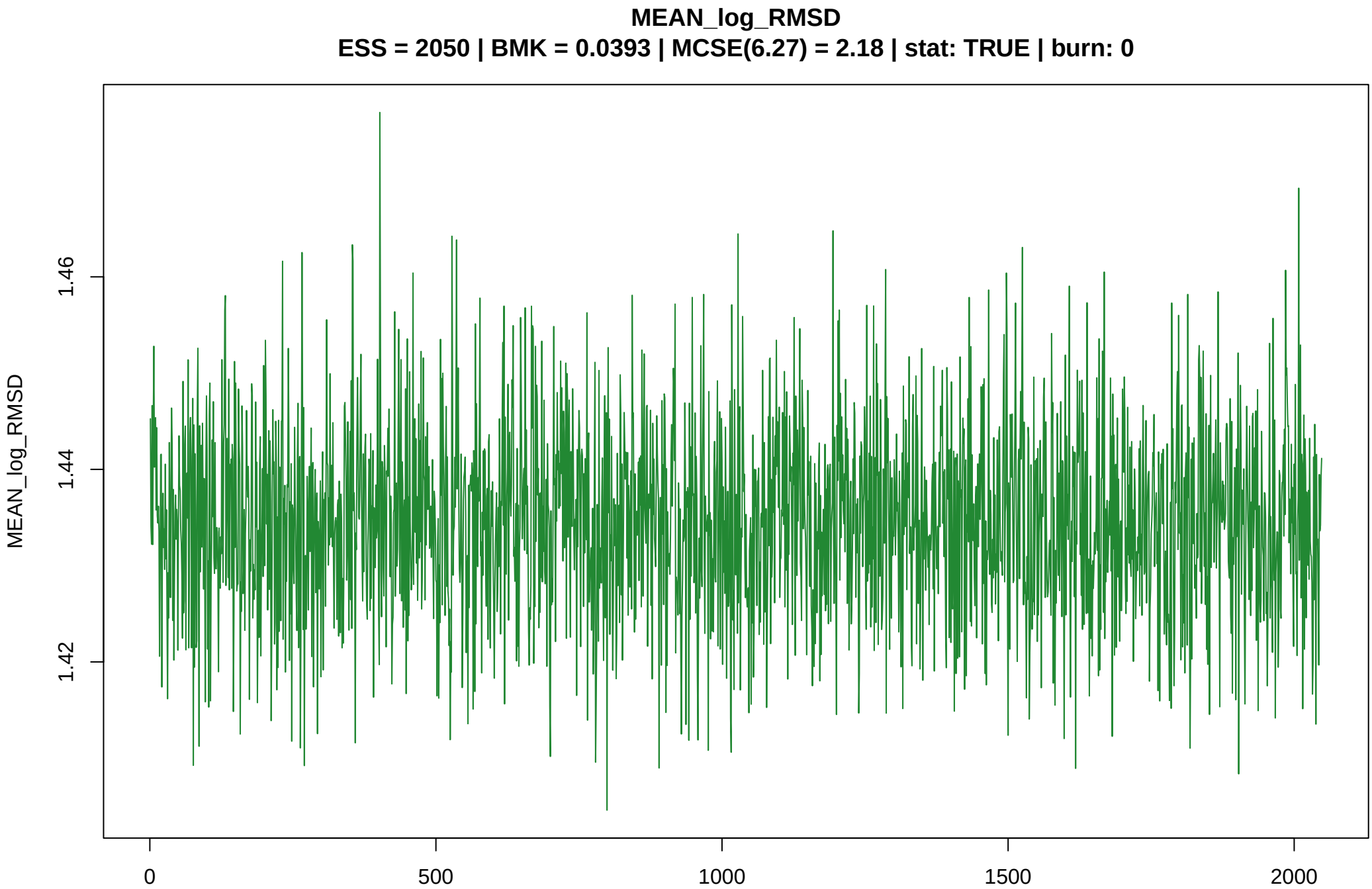

Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1224
Q3_template_HeavyAtomCount
34.0
33.8
33.6
33.4
33.2
33.0
0
500
1000
1500
2000

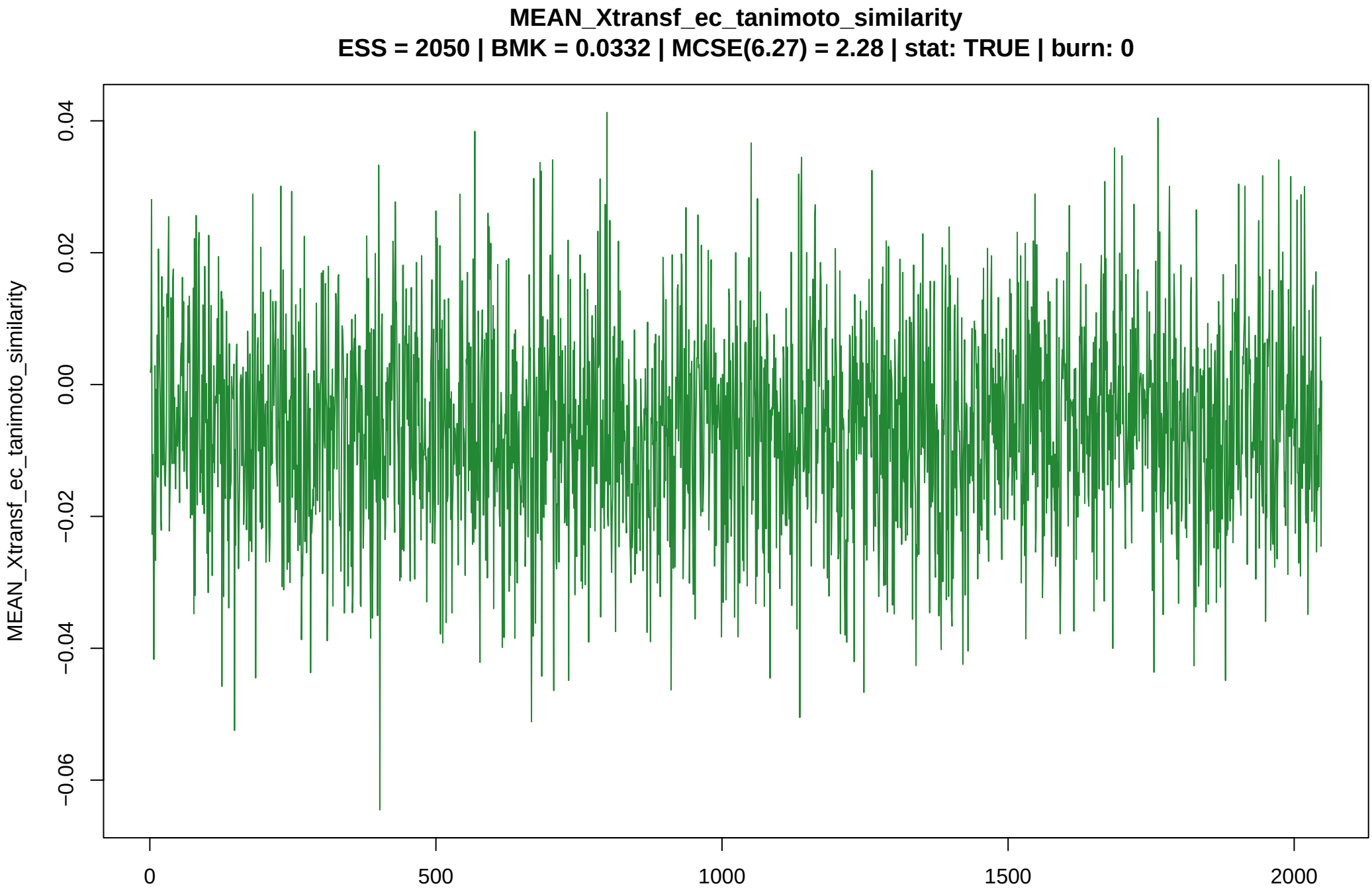

Q3_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_docked_NumHAcceptors
1.5
2.0
2.5
0
500
1000
1500
2000

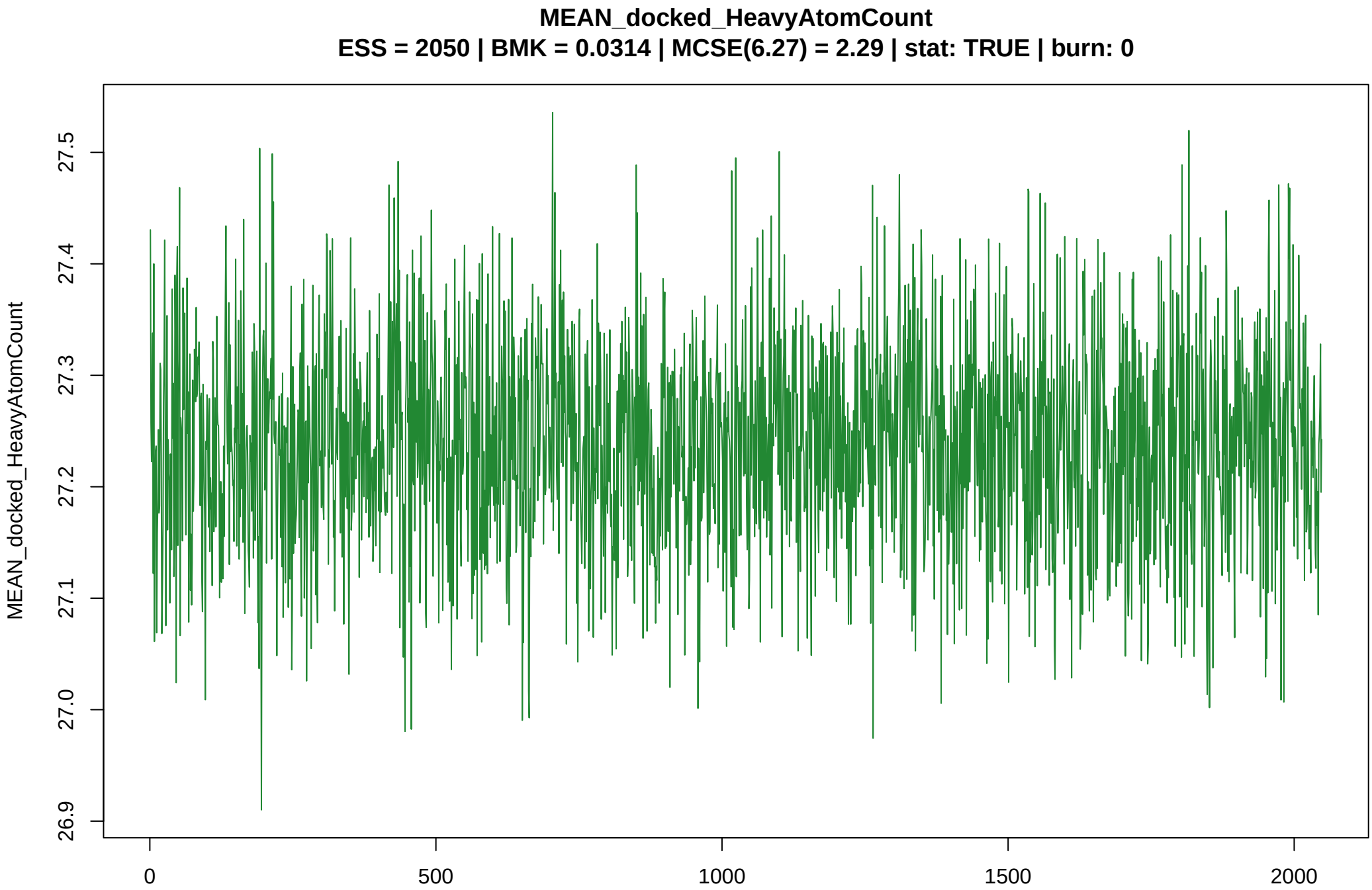

Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632
Q3_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

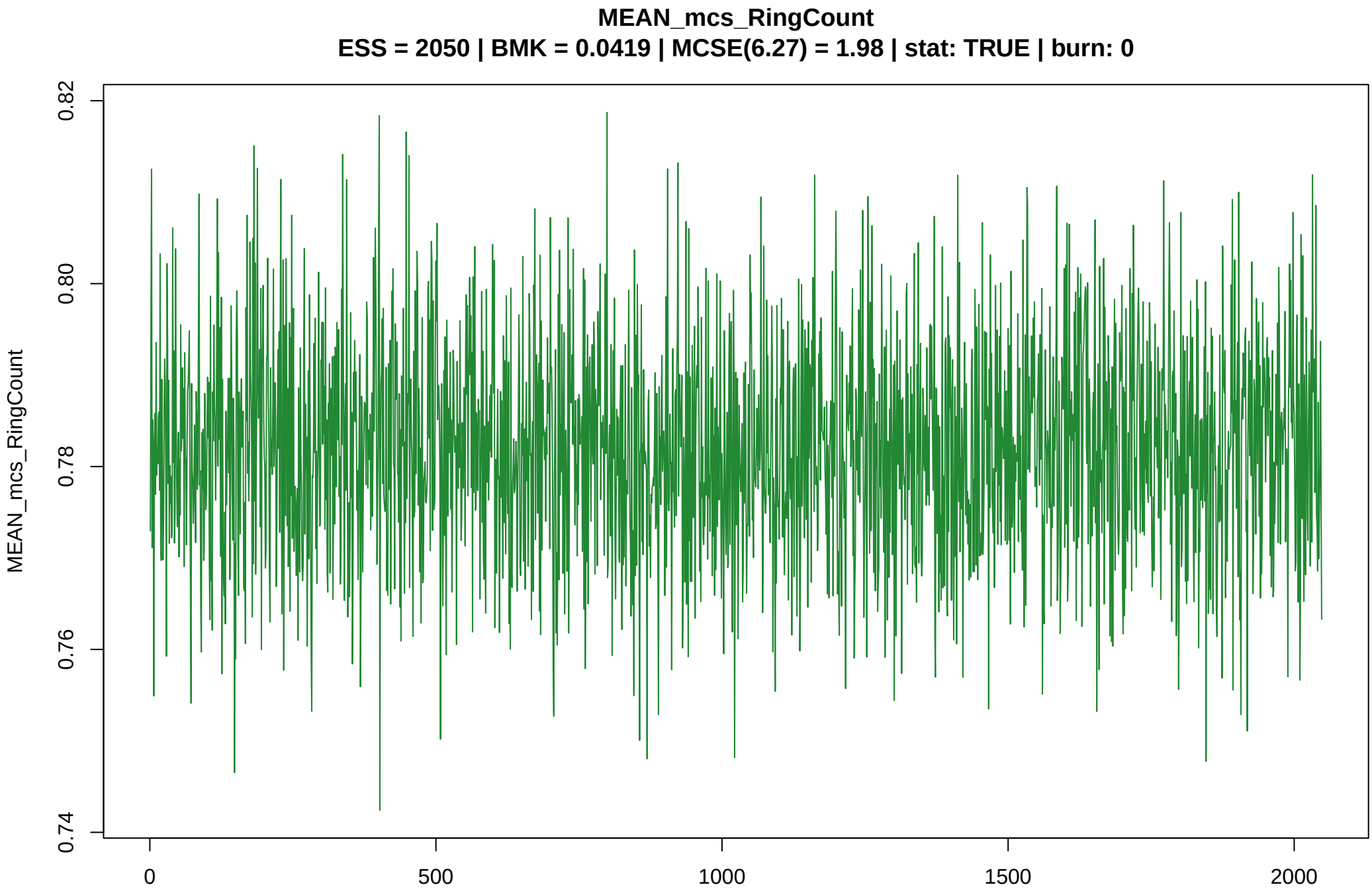

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

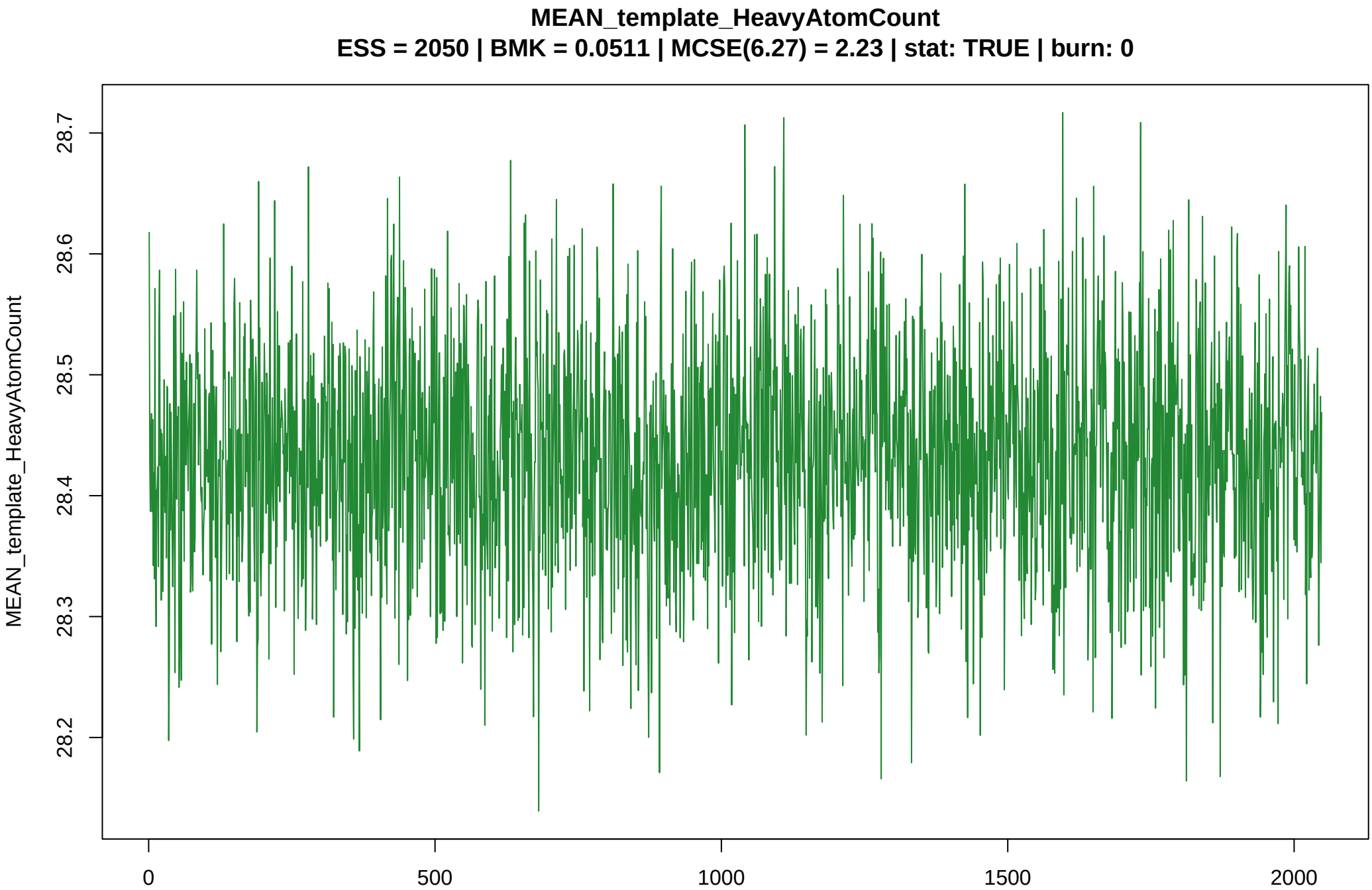

Dcov
ESS = 2050 | BMK = 0.0422 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
Dcov
2
1
0
−1
−2
0
500
1000
1500
2000

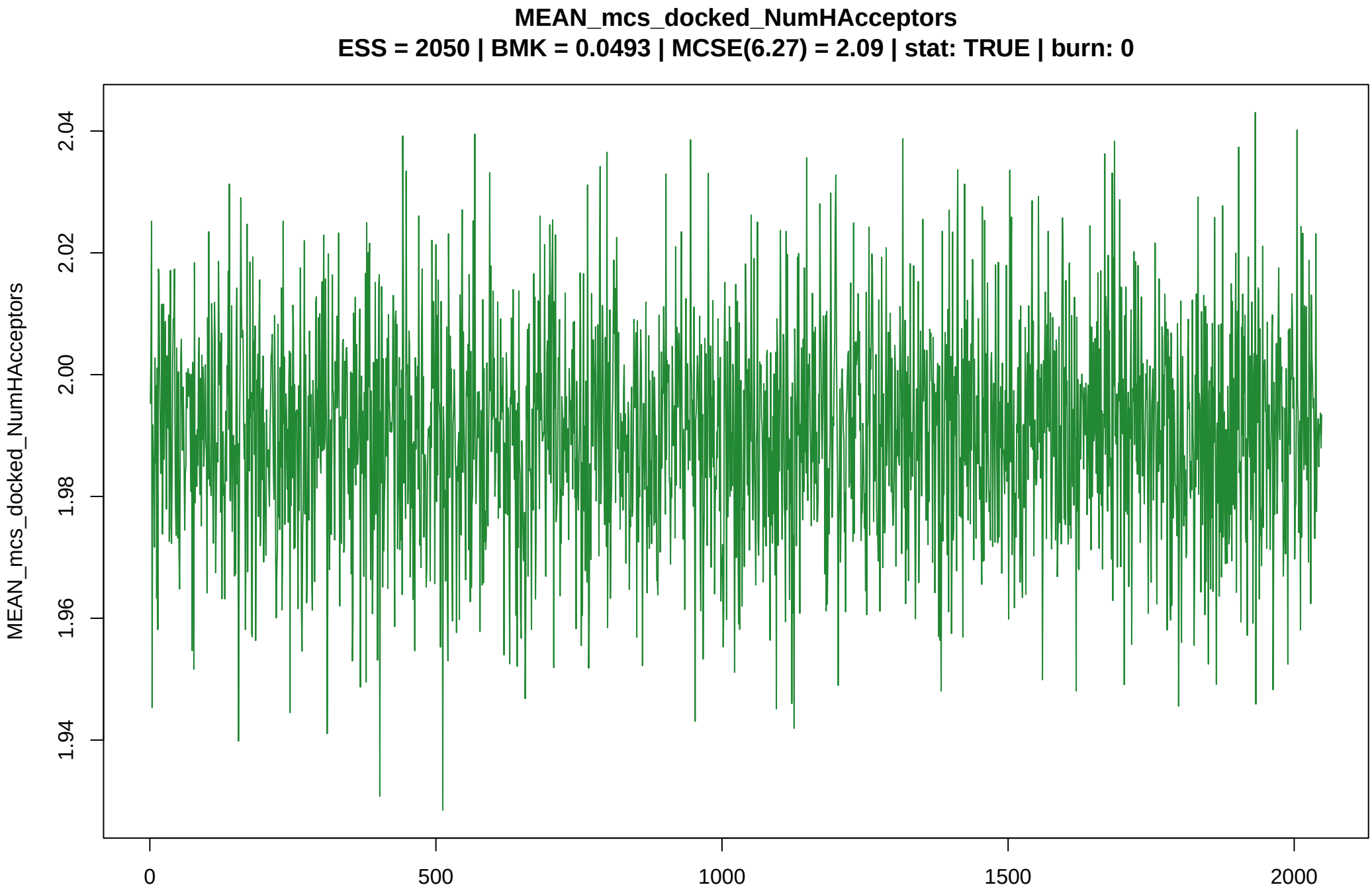

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0393 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.42
1.44
1.46
0
500
1000
1500
2000

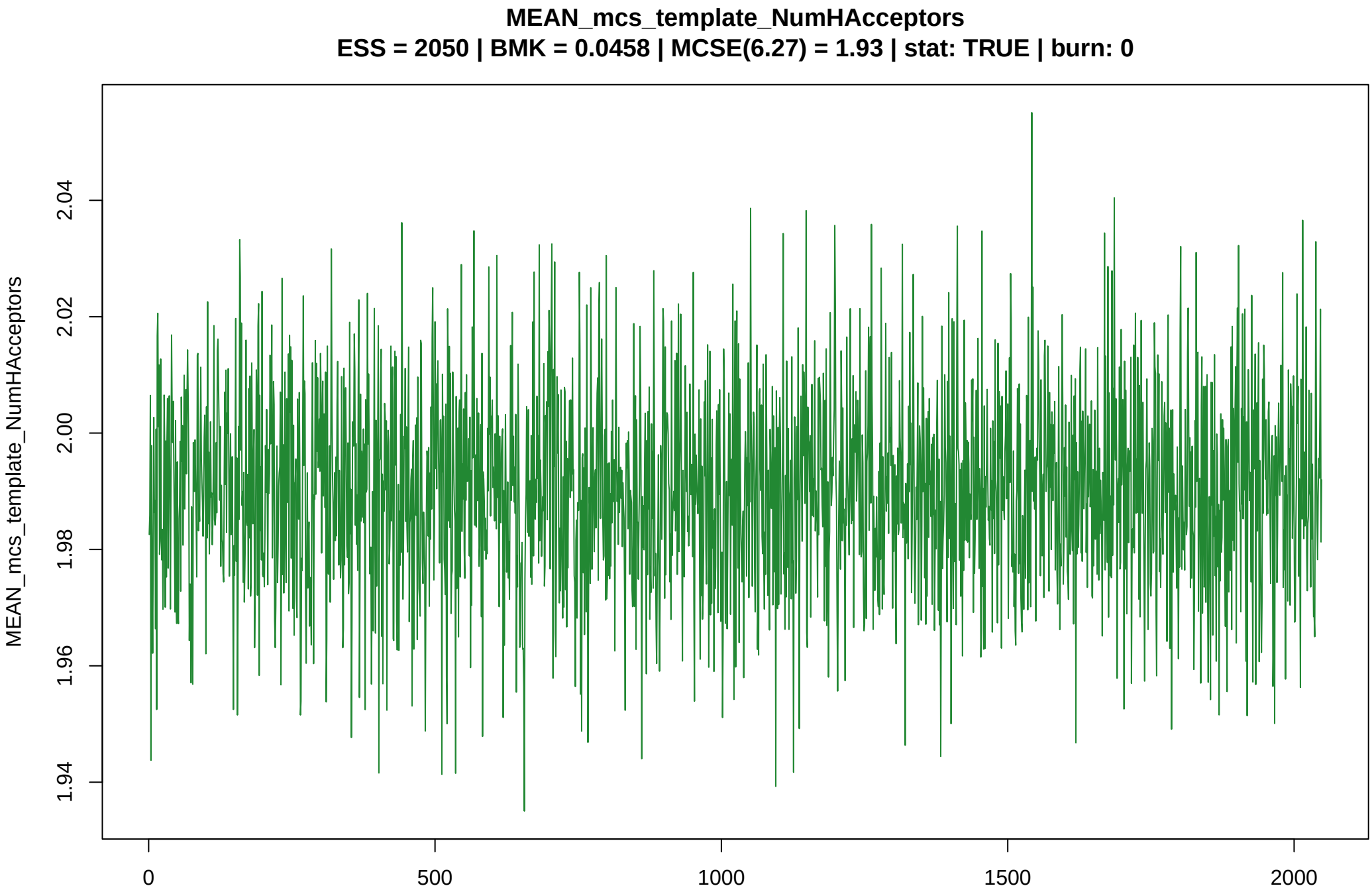

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0332 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
500
1000
1500
2000

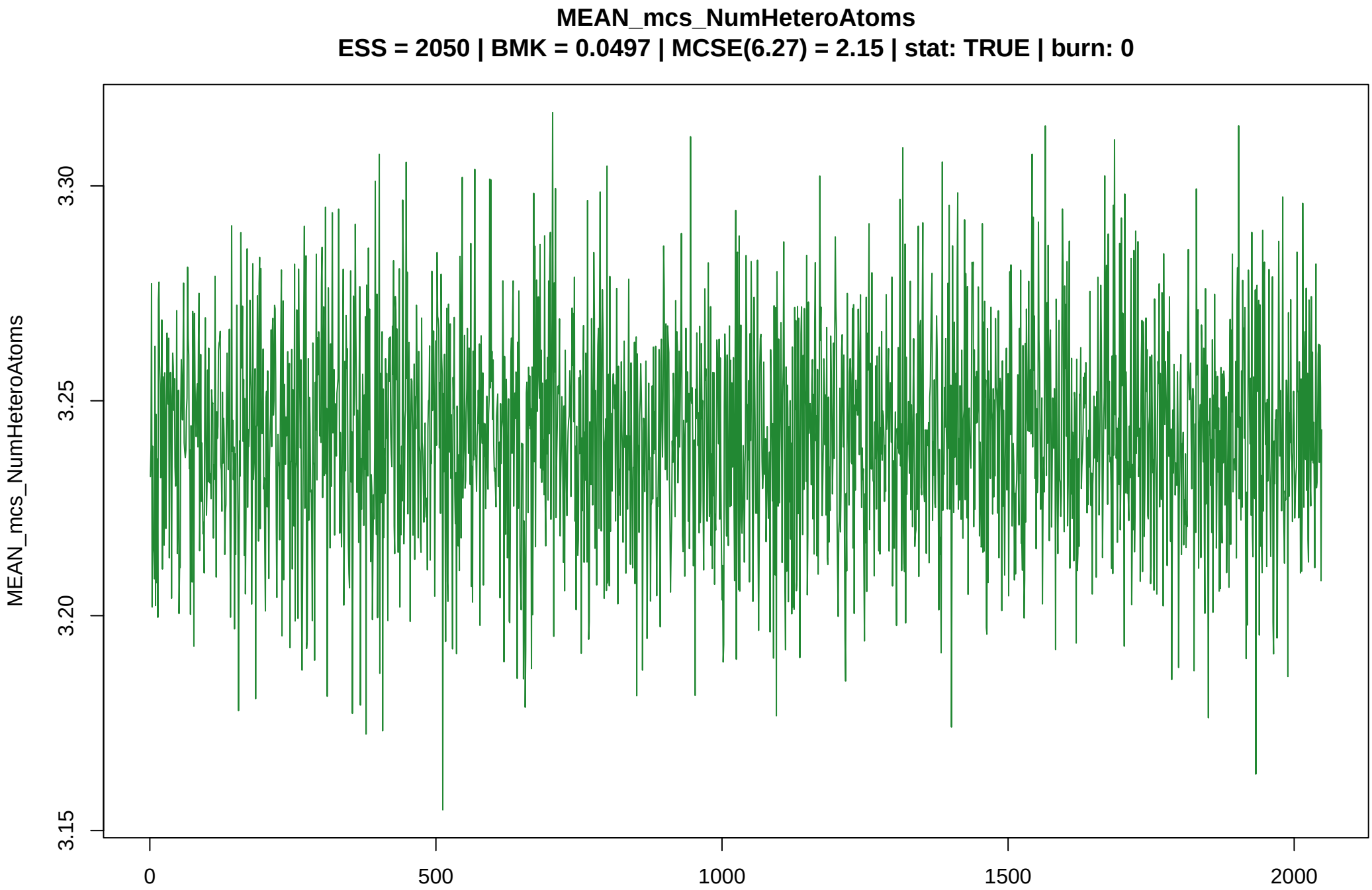

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0314 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
26.9
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

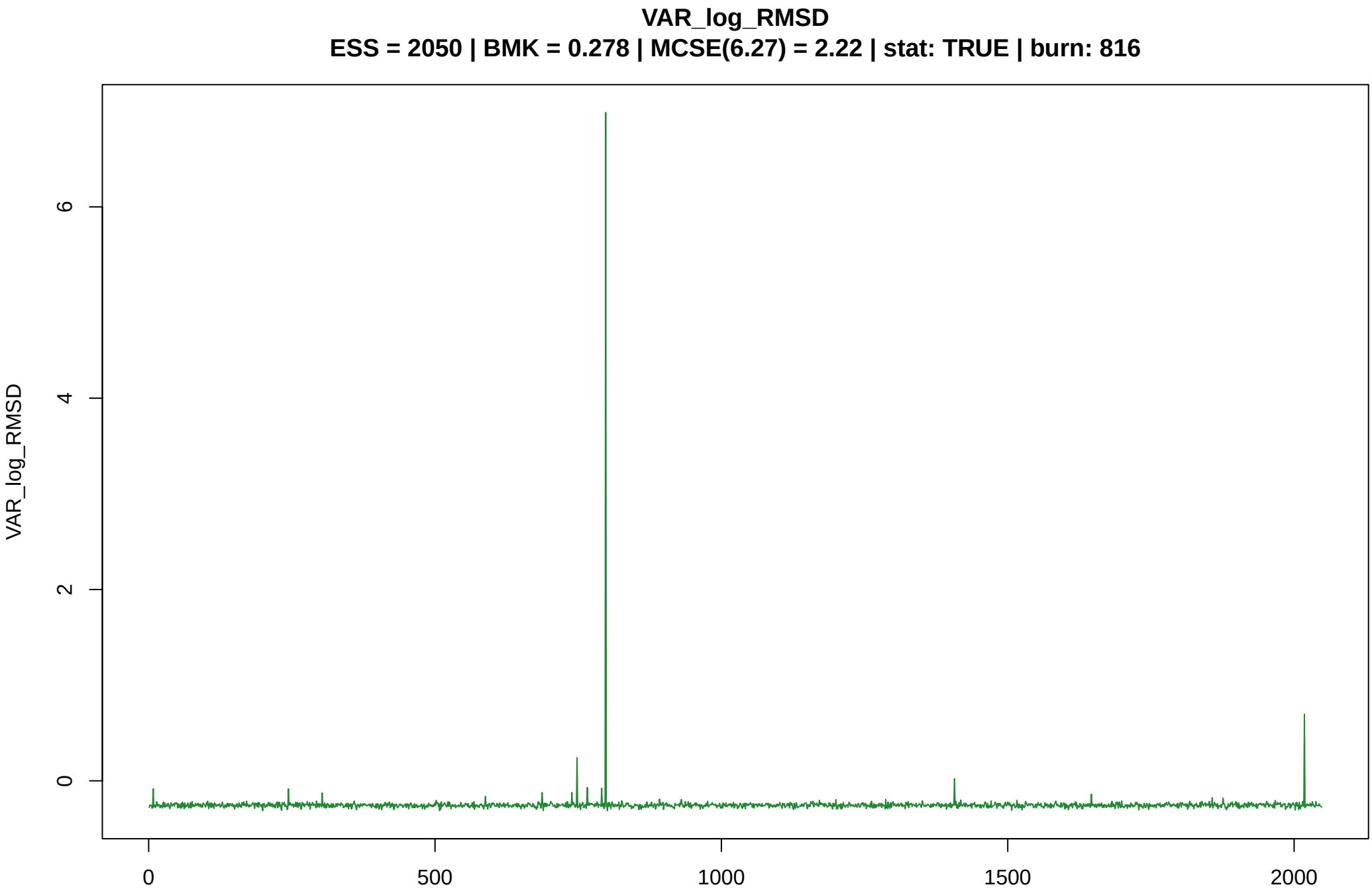

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

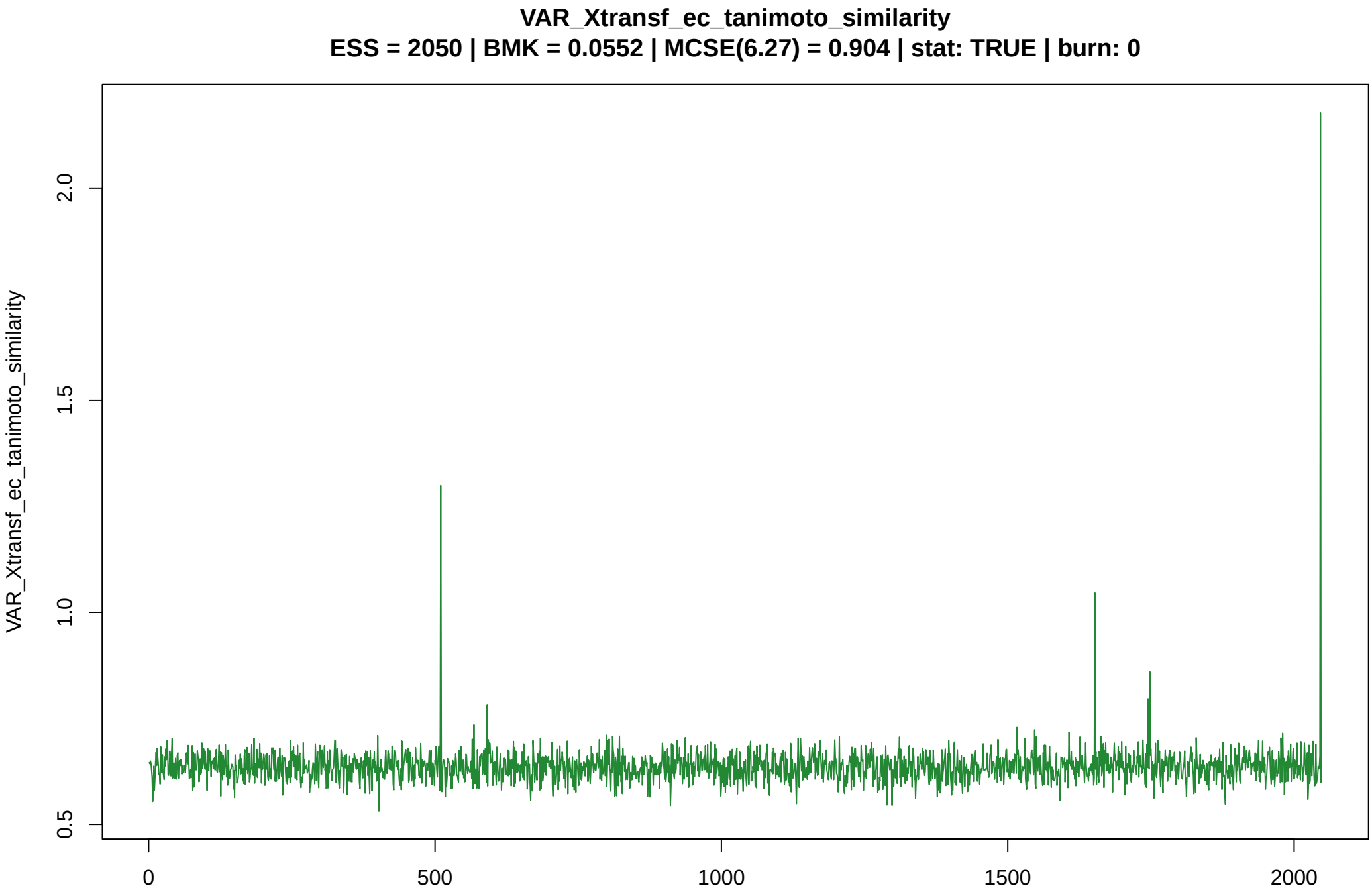

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0511 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

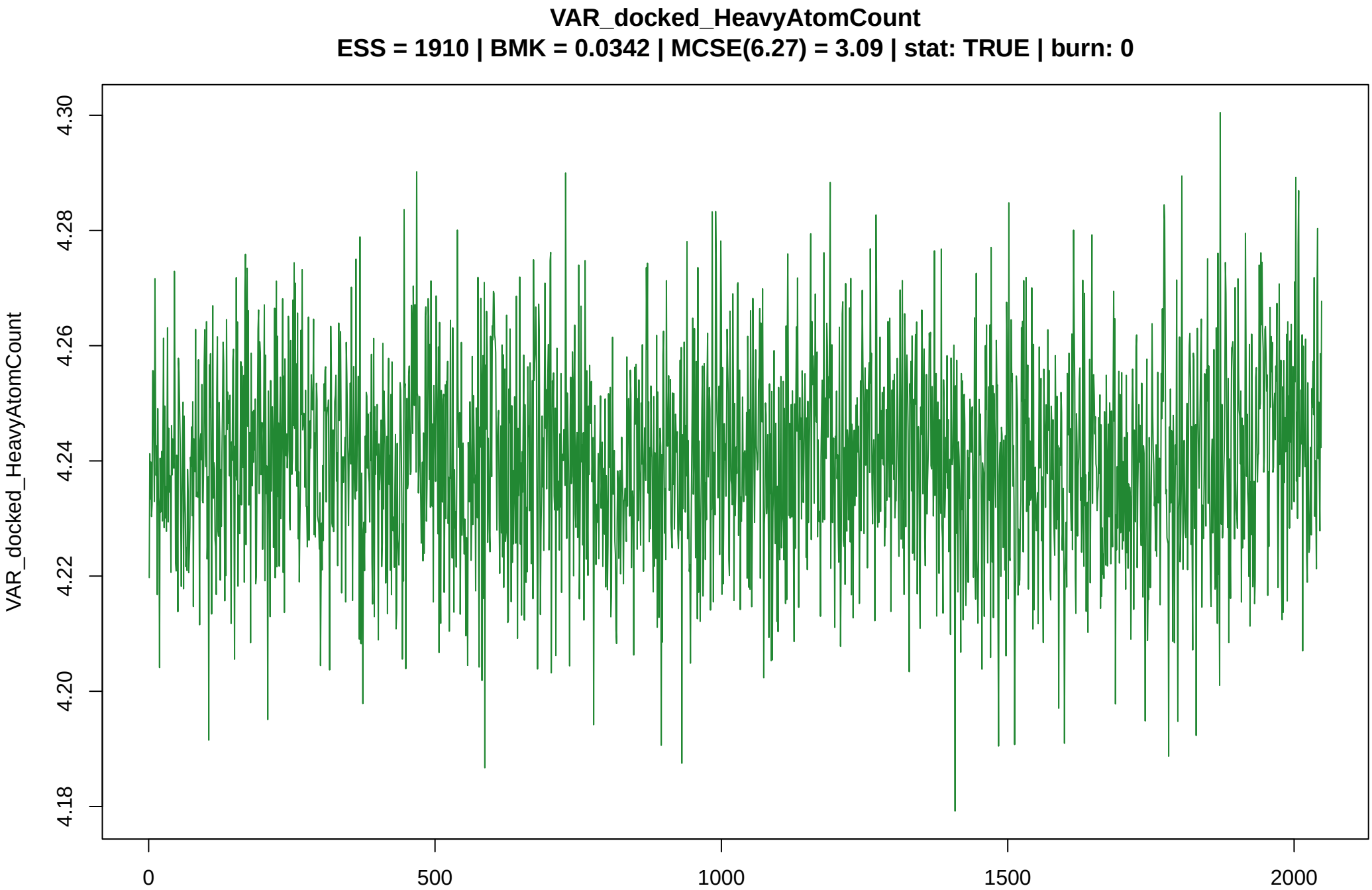

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0493 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

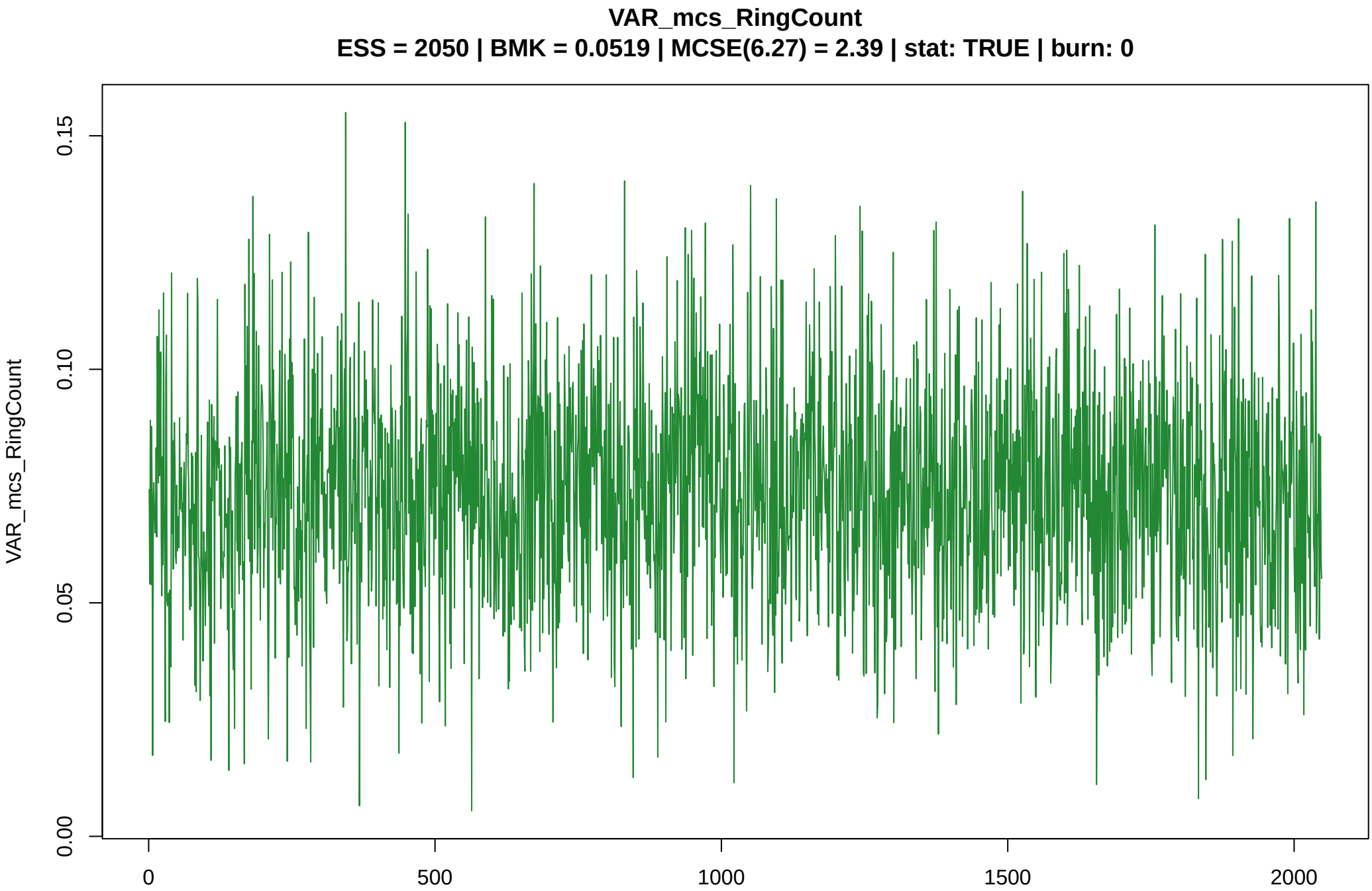

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

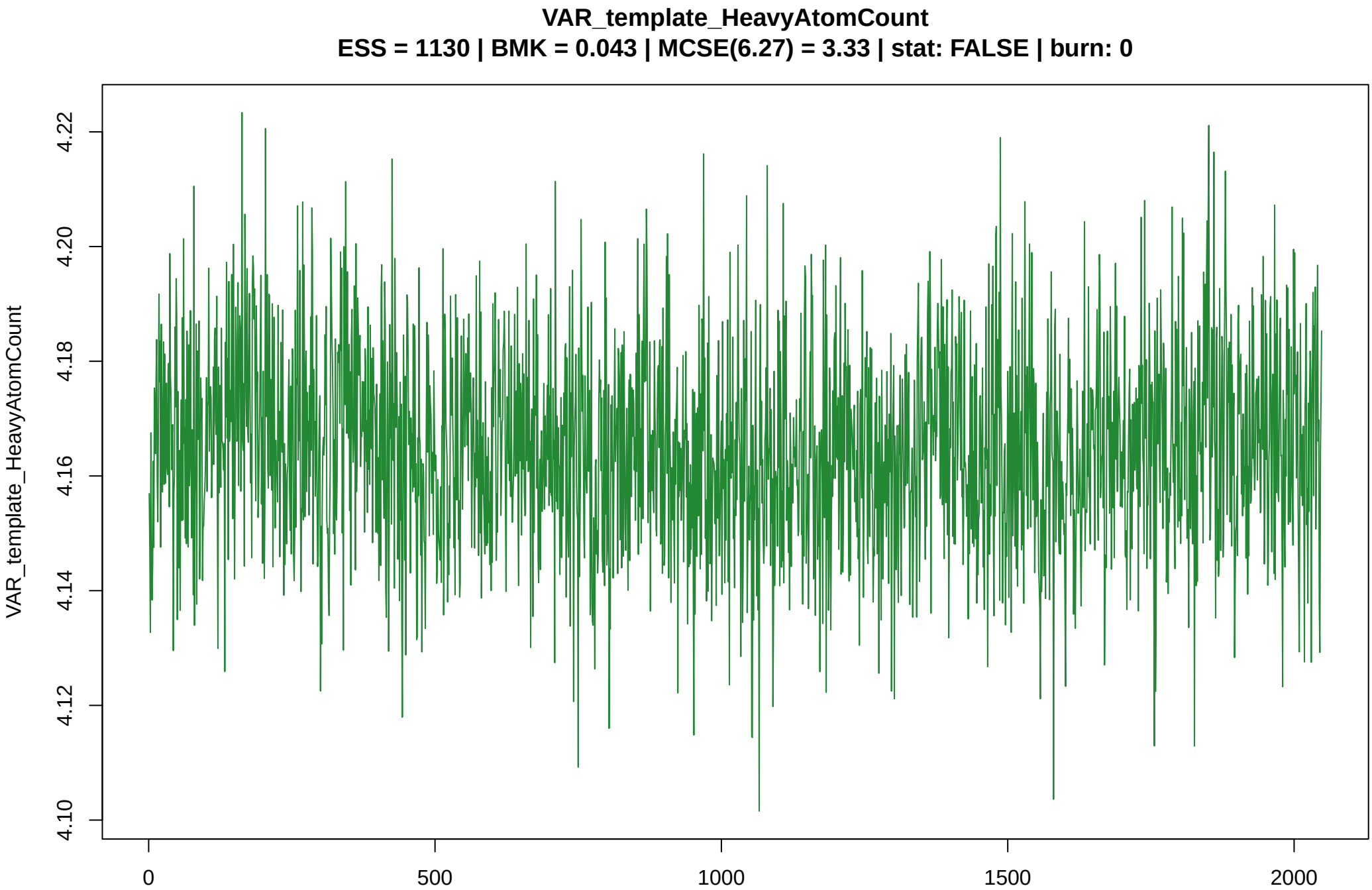

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0497 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.15
3.20
3.25
3.30
0
500
1000
1500
2000

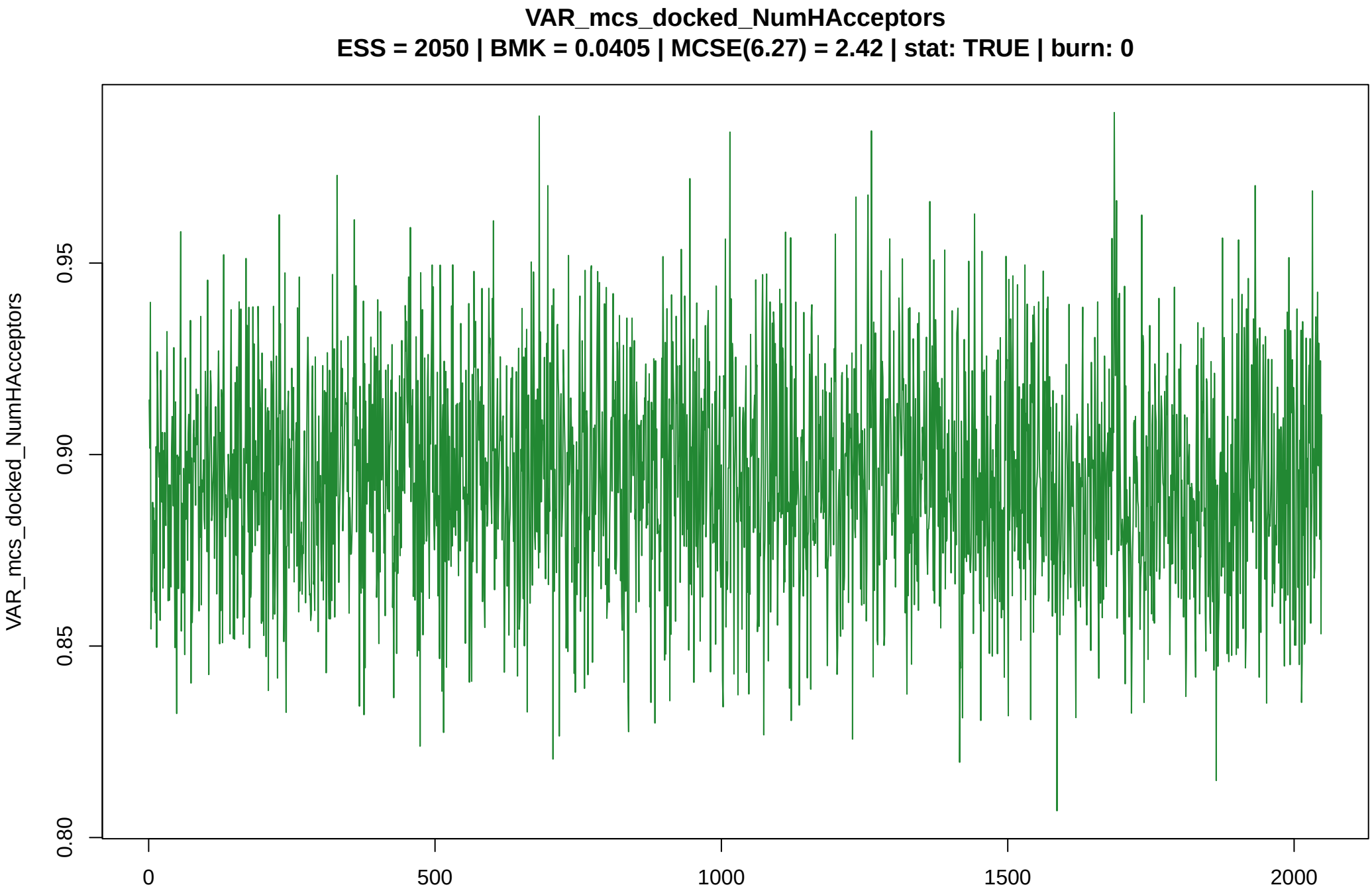

VAR_log_RMSD
ESS = 2050 | BMK = 0.278 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 816
VAR_log_RMSD
0
2
4
6
0
500
1000
1500
2000

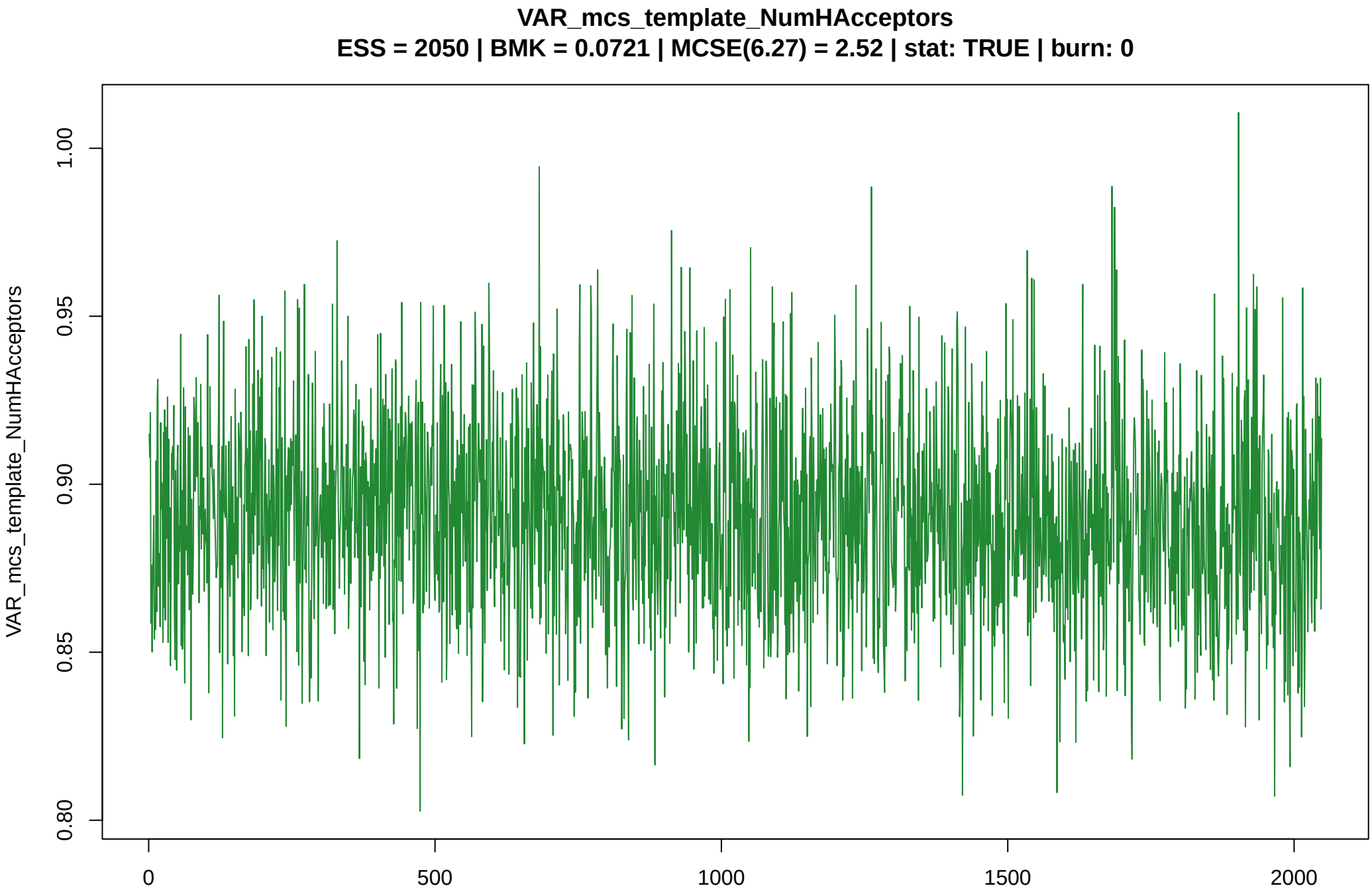

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0552 | MCSE(6.27) = 0.904 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
0.5
1.0
1.5
2.0
0
500
1000
1500
2000

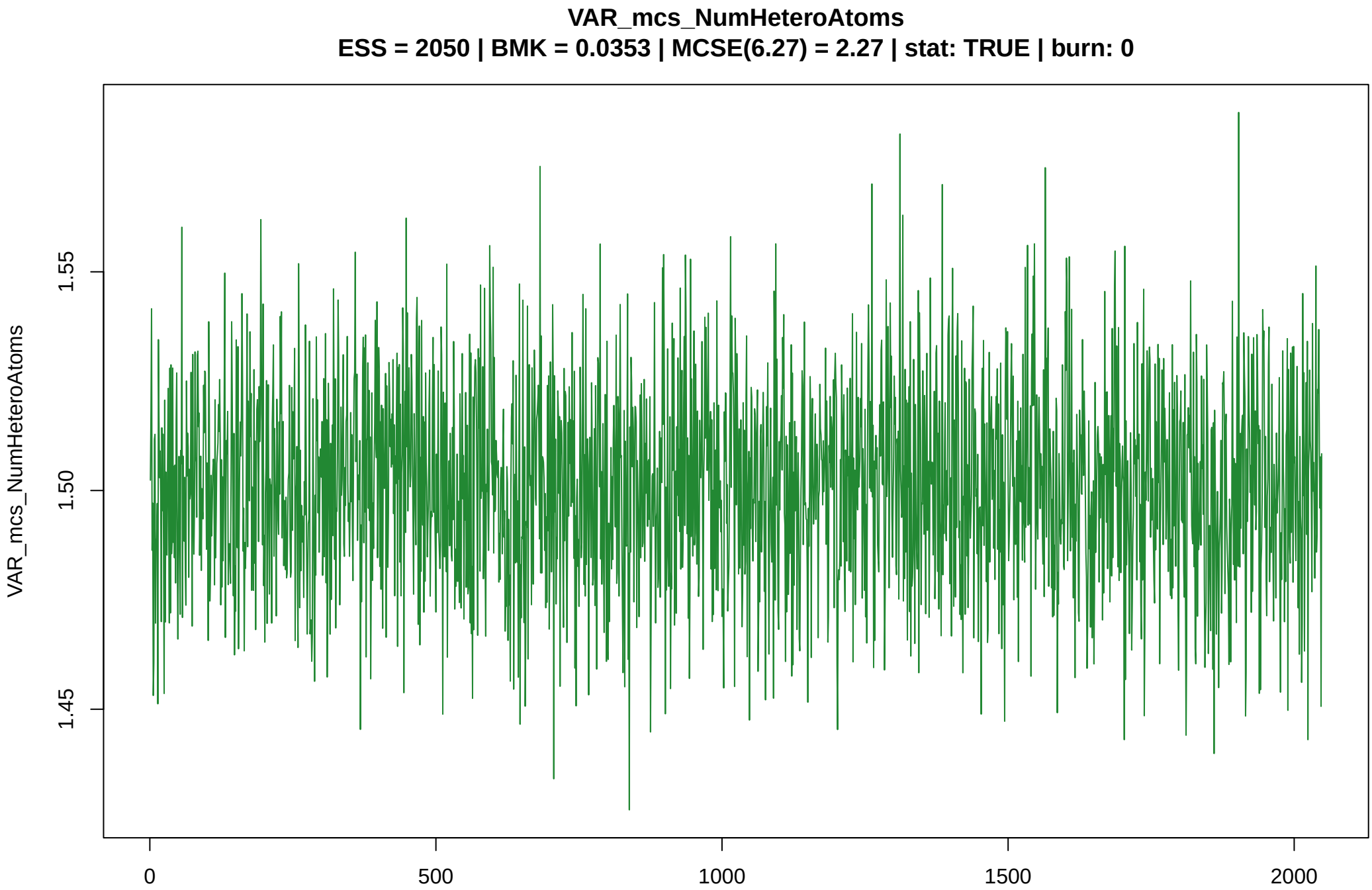

VAR_docked_HeavyAtomCount
ESS = 1910 | BMK = 0.0342 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
4.30
0
500
1000
1500
2000

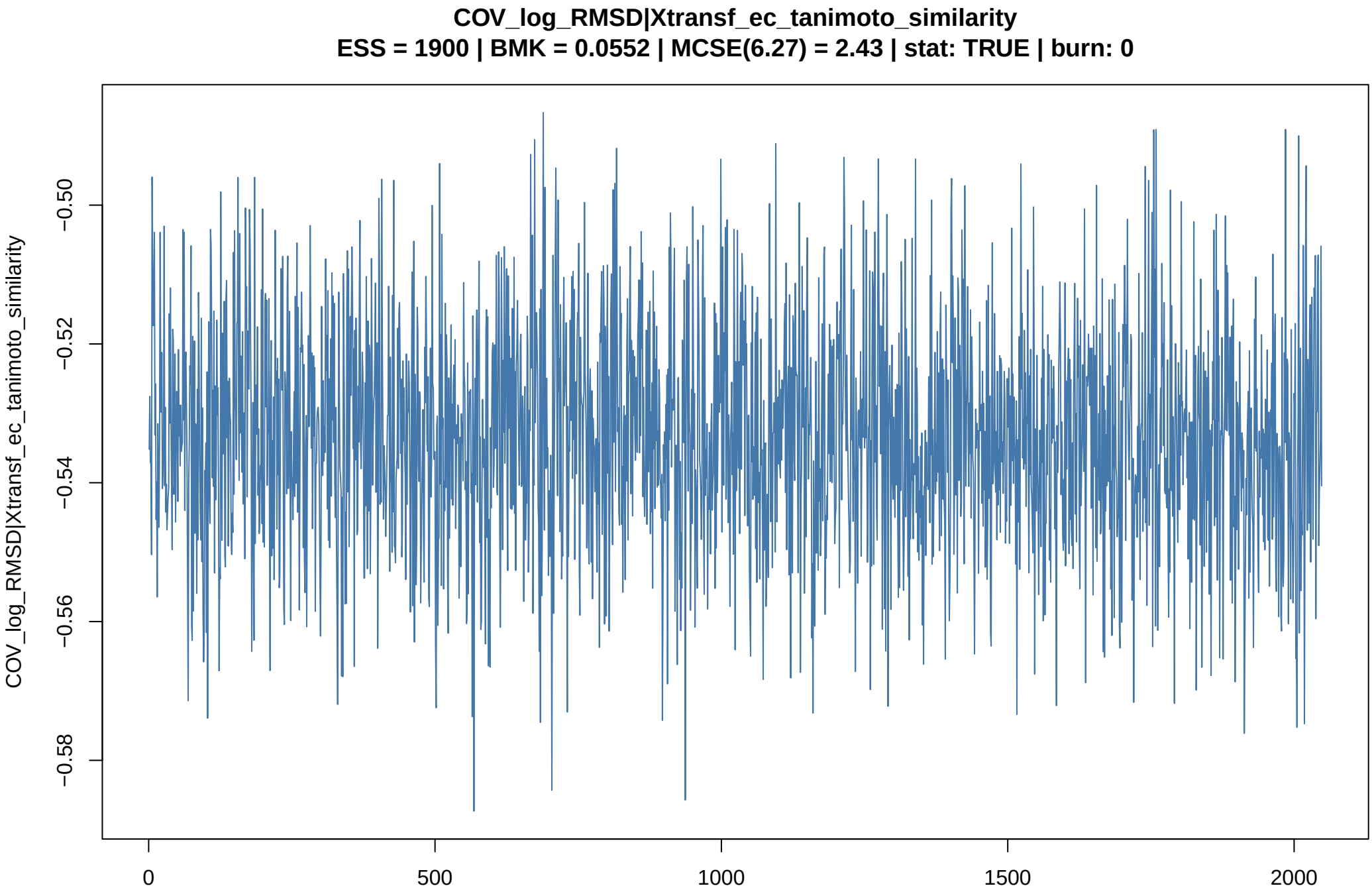

VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0519 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0
VAR_mcs_RingCount
0.00
0.05
0.10
0.15
0
500
1000
1500
2000

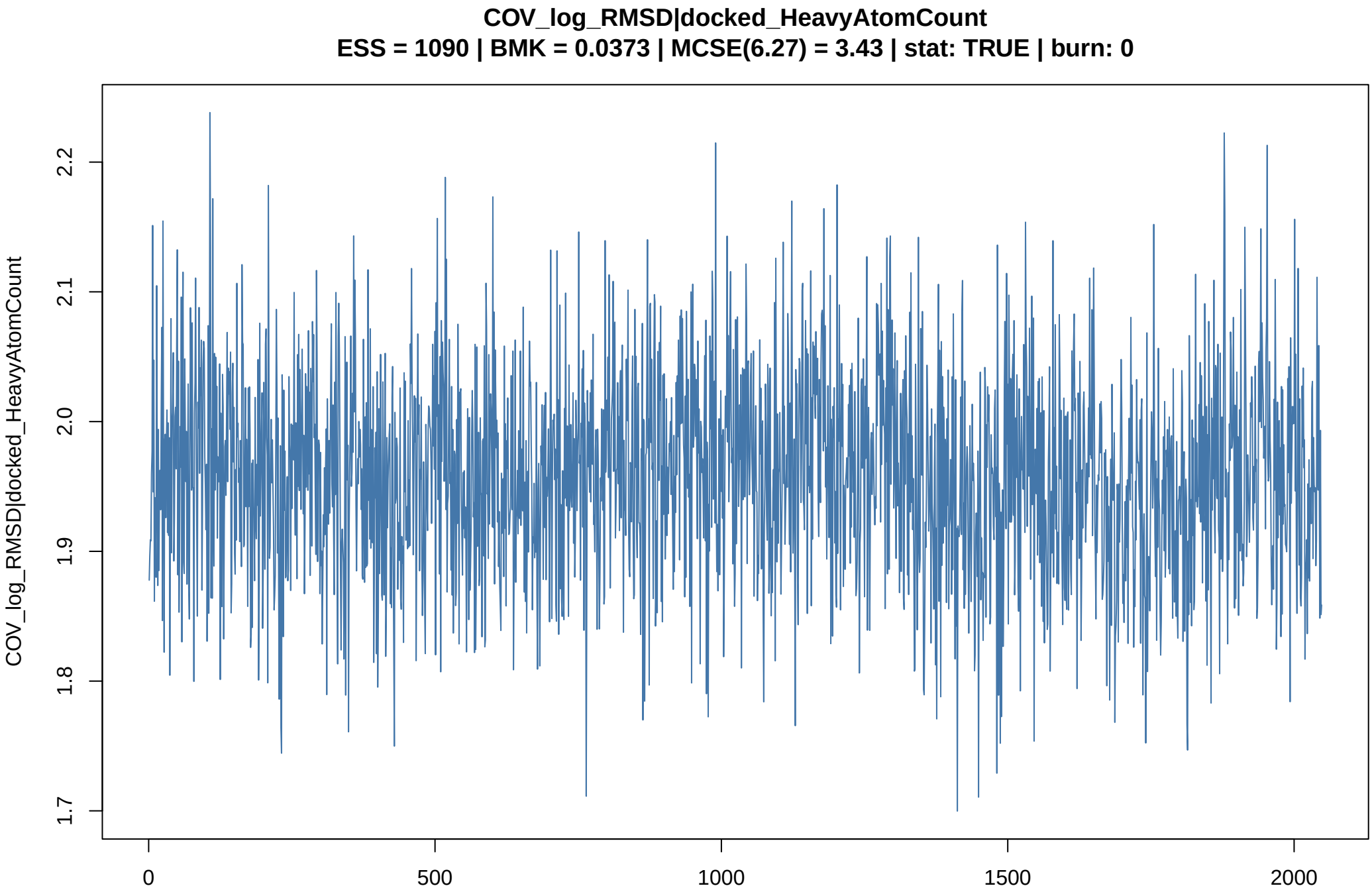

VAR_template_HeavyAtomCount
ESS = 1130 | BMK = 0.043 | MCSE(6.27) = 3.33 | stat: FALSE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
4.22
0
500
1000
1500
2000

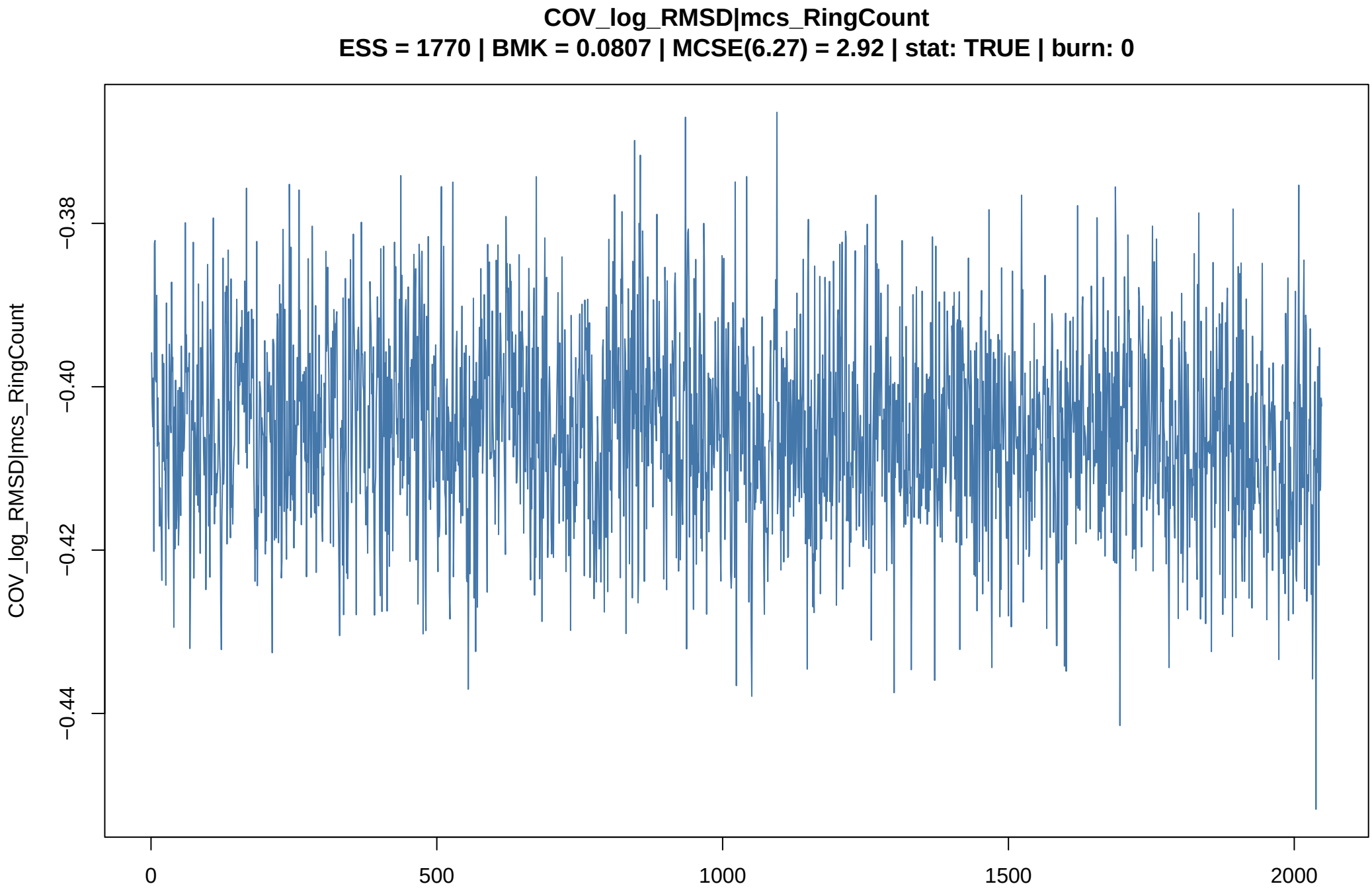

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0405 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

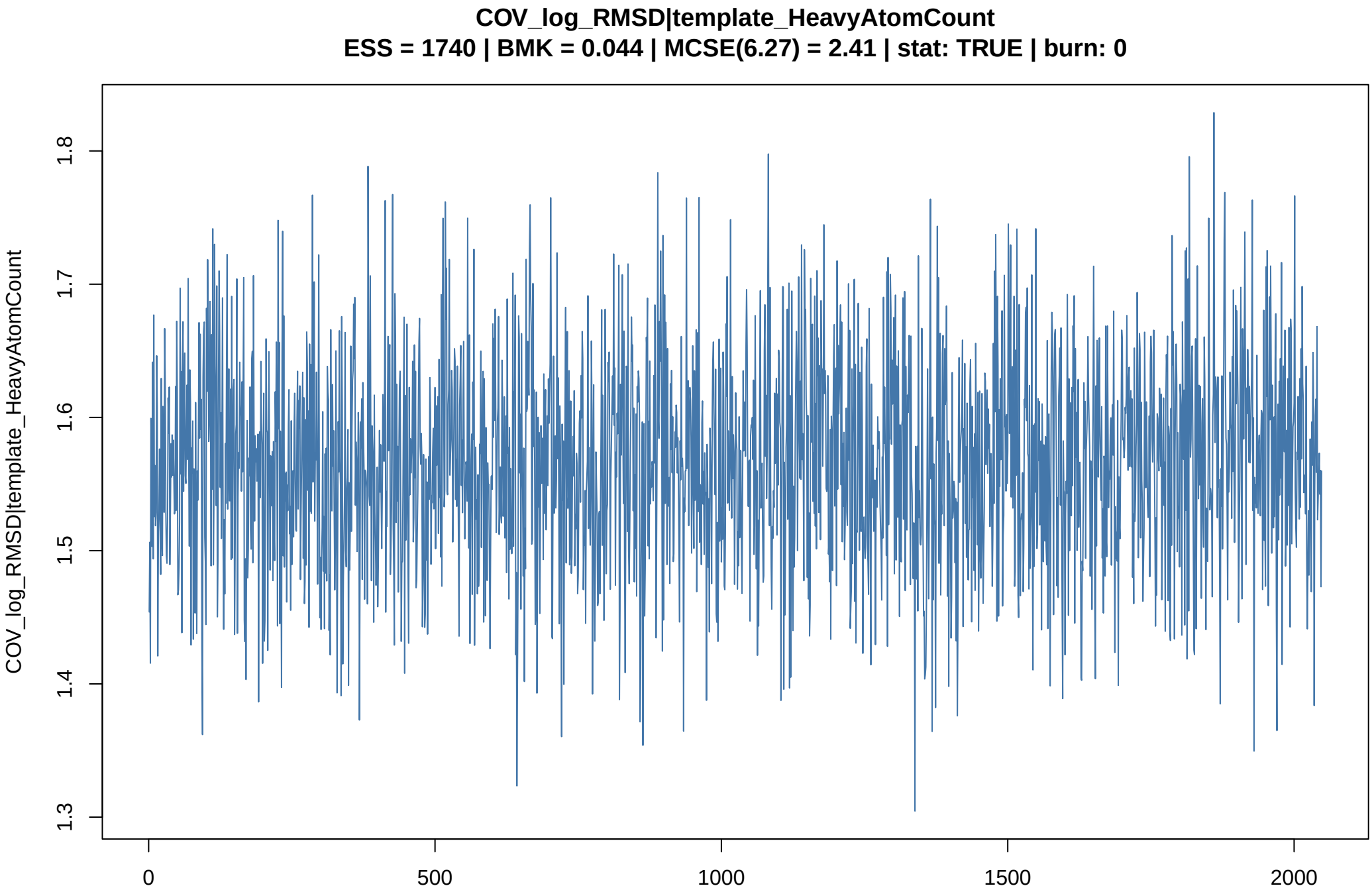

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0721 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
1.00
0.95
0.90
0.85
0.80
0
500
1000
1500
2000

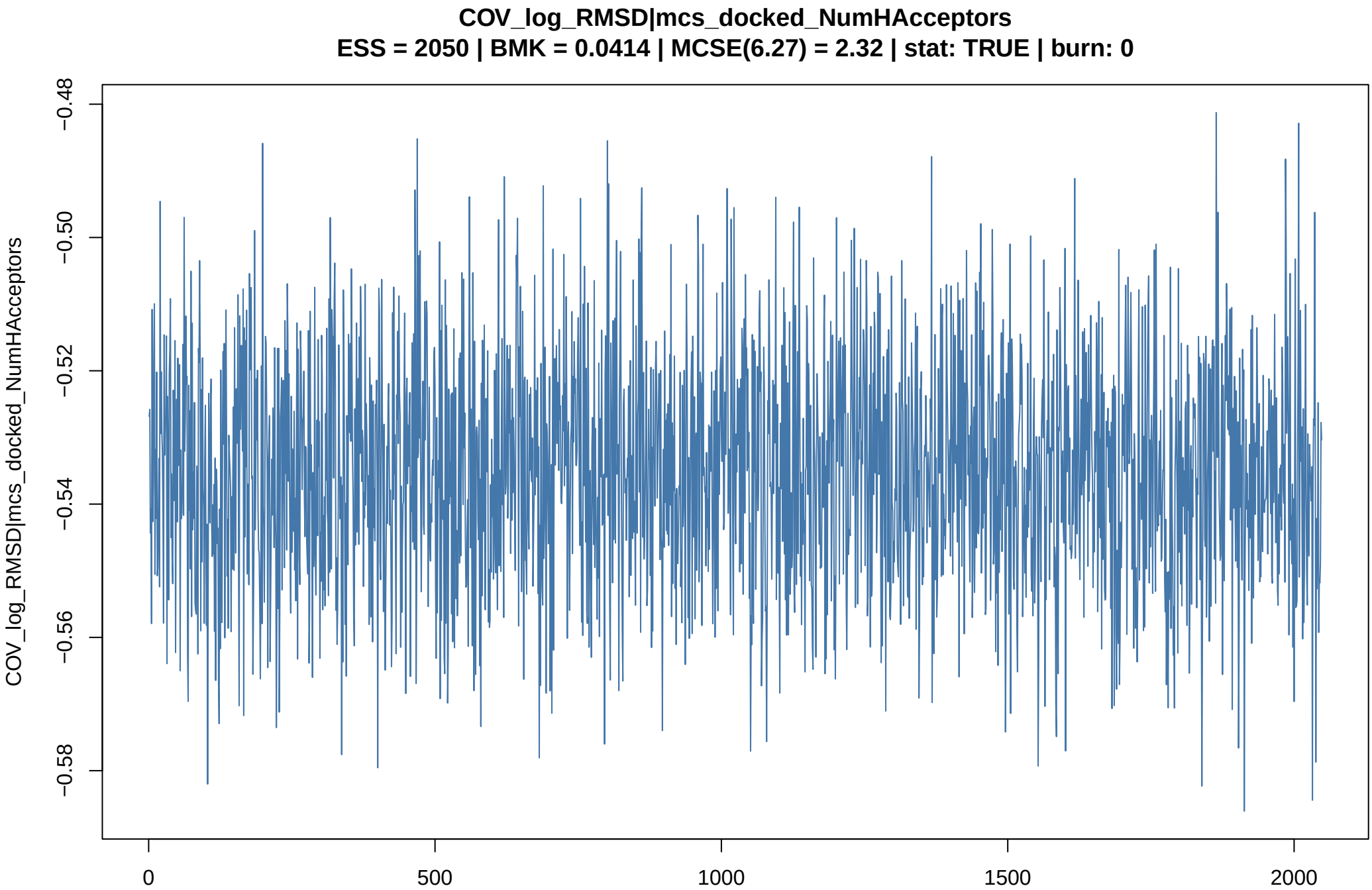

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0353 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

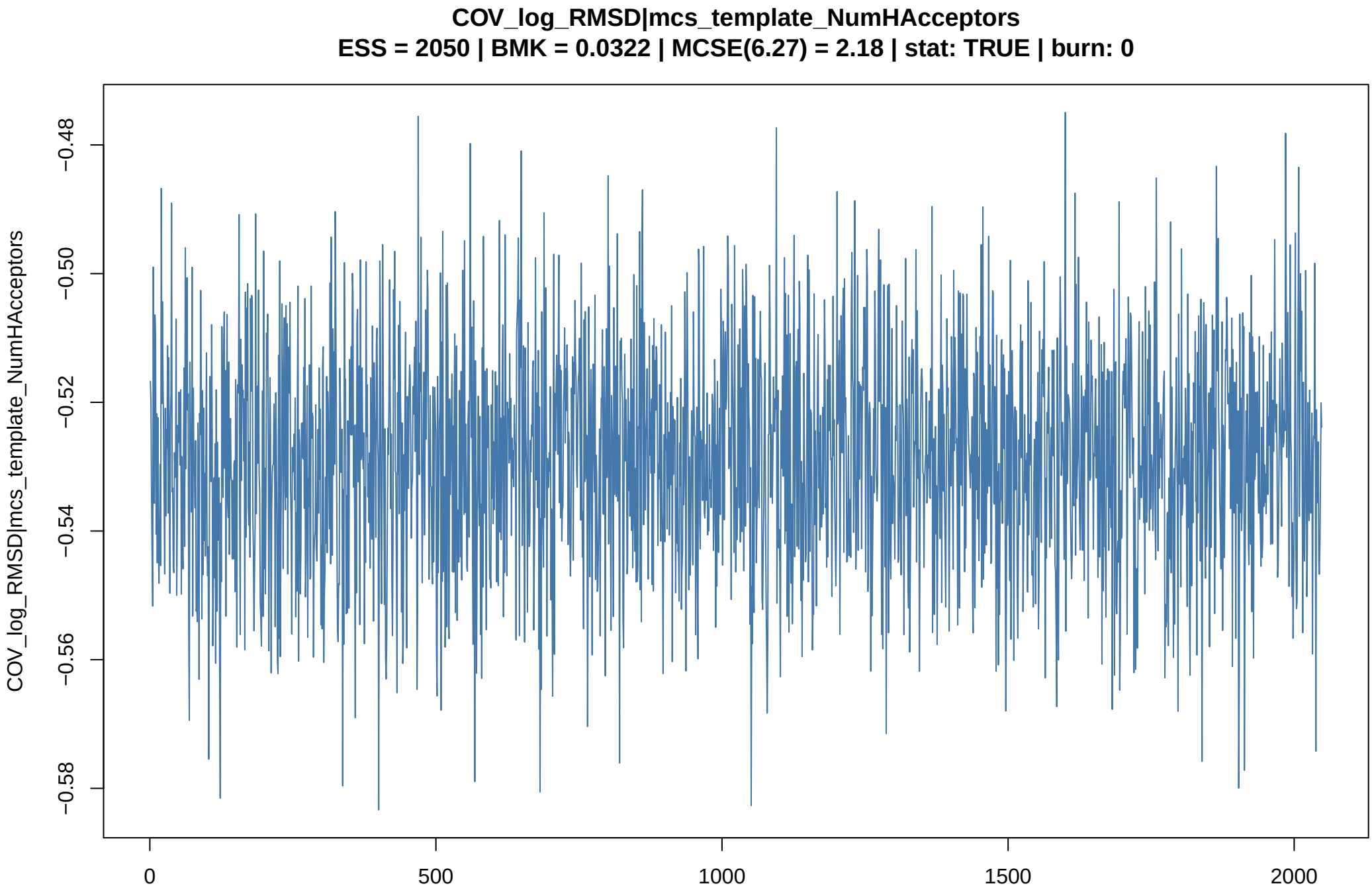

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1900 | BMK = 0.0552 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

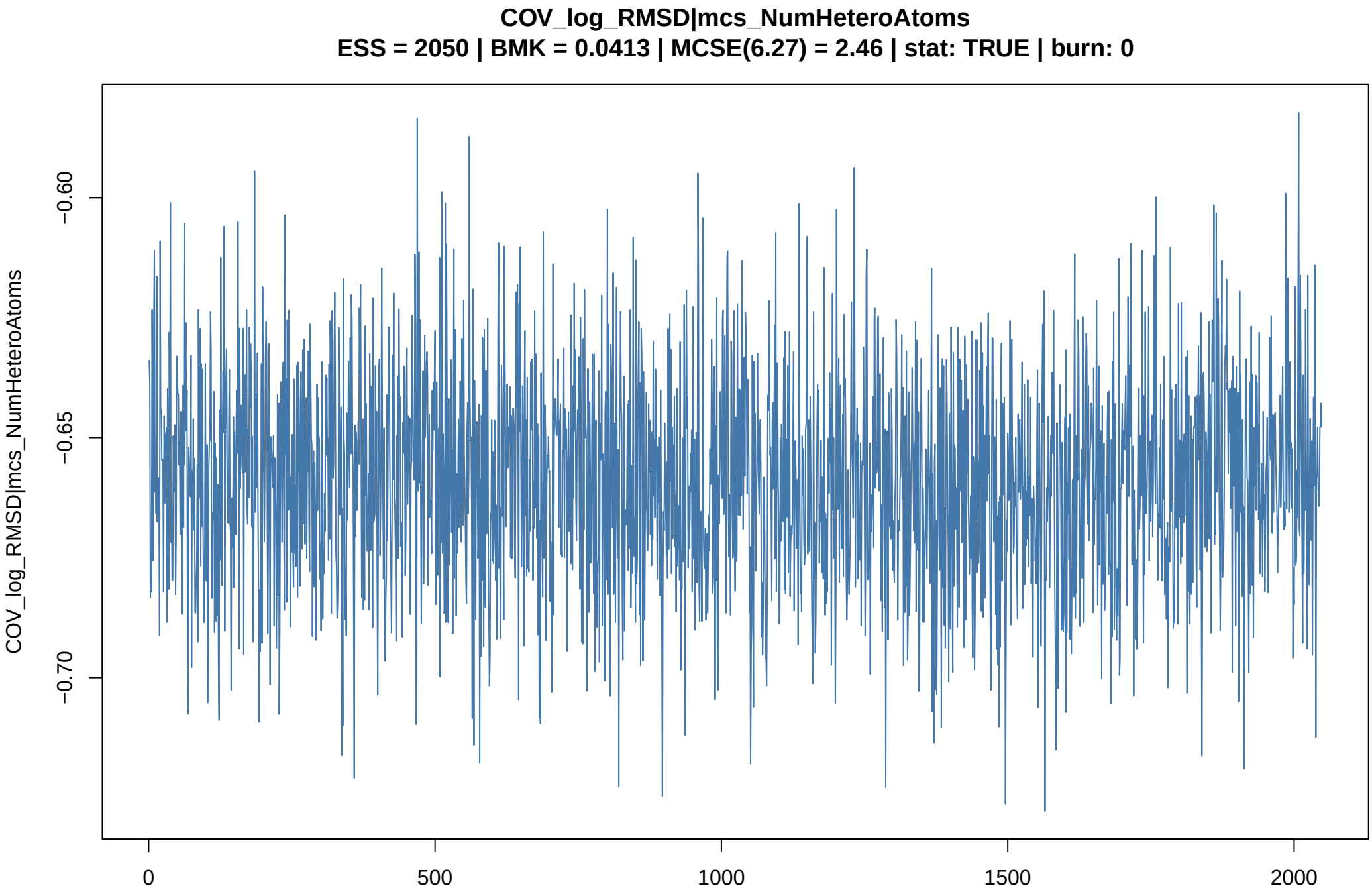

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1090 | BMK = 0.0373 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.7
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

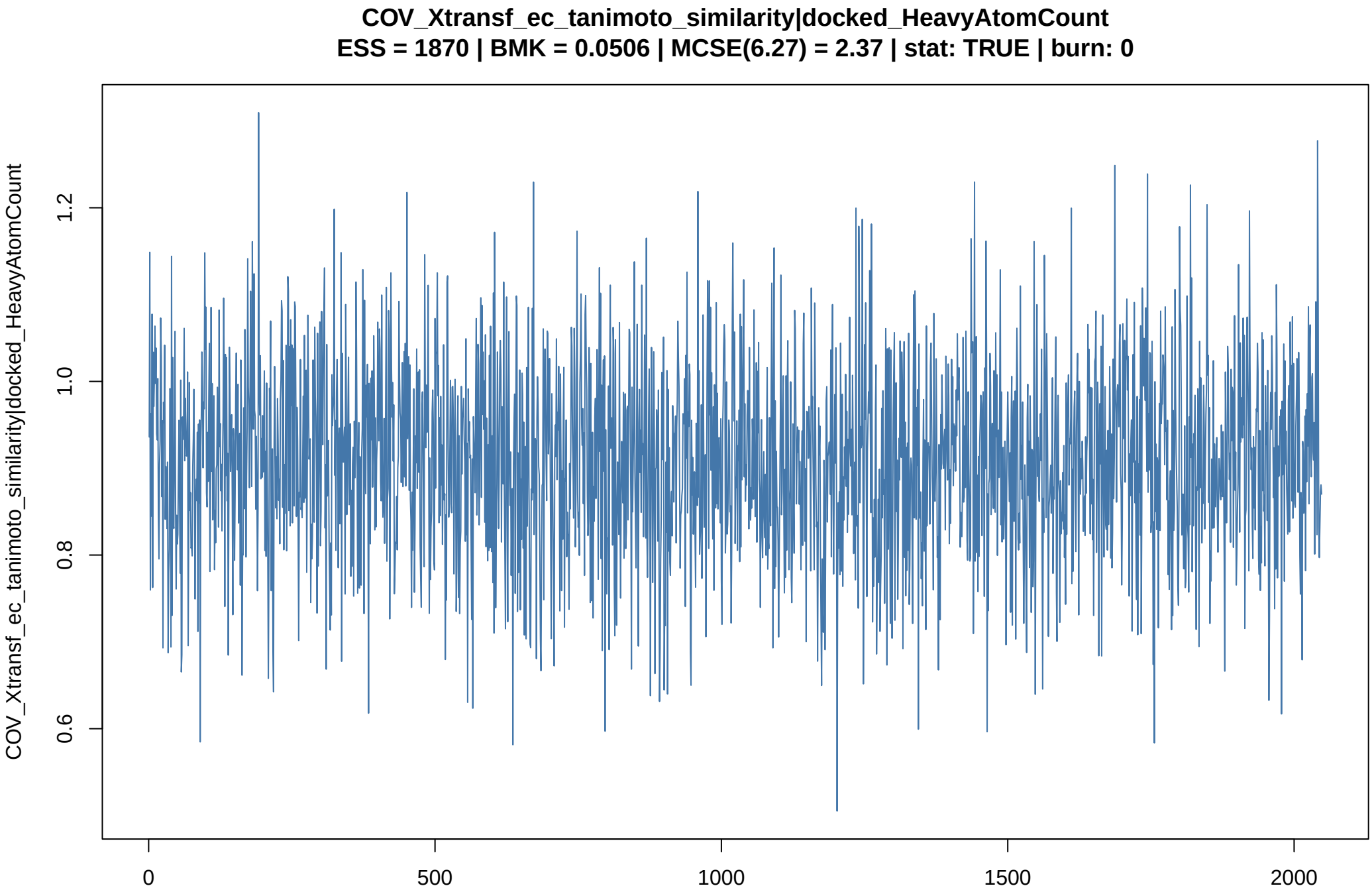

COV_log_RMSD|mcs_RingCount
ESS = 1770 | BMK = 0.0807 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.38
−0.40
−0.42
−0.44
0
500
1000
1500
2000

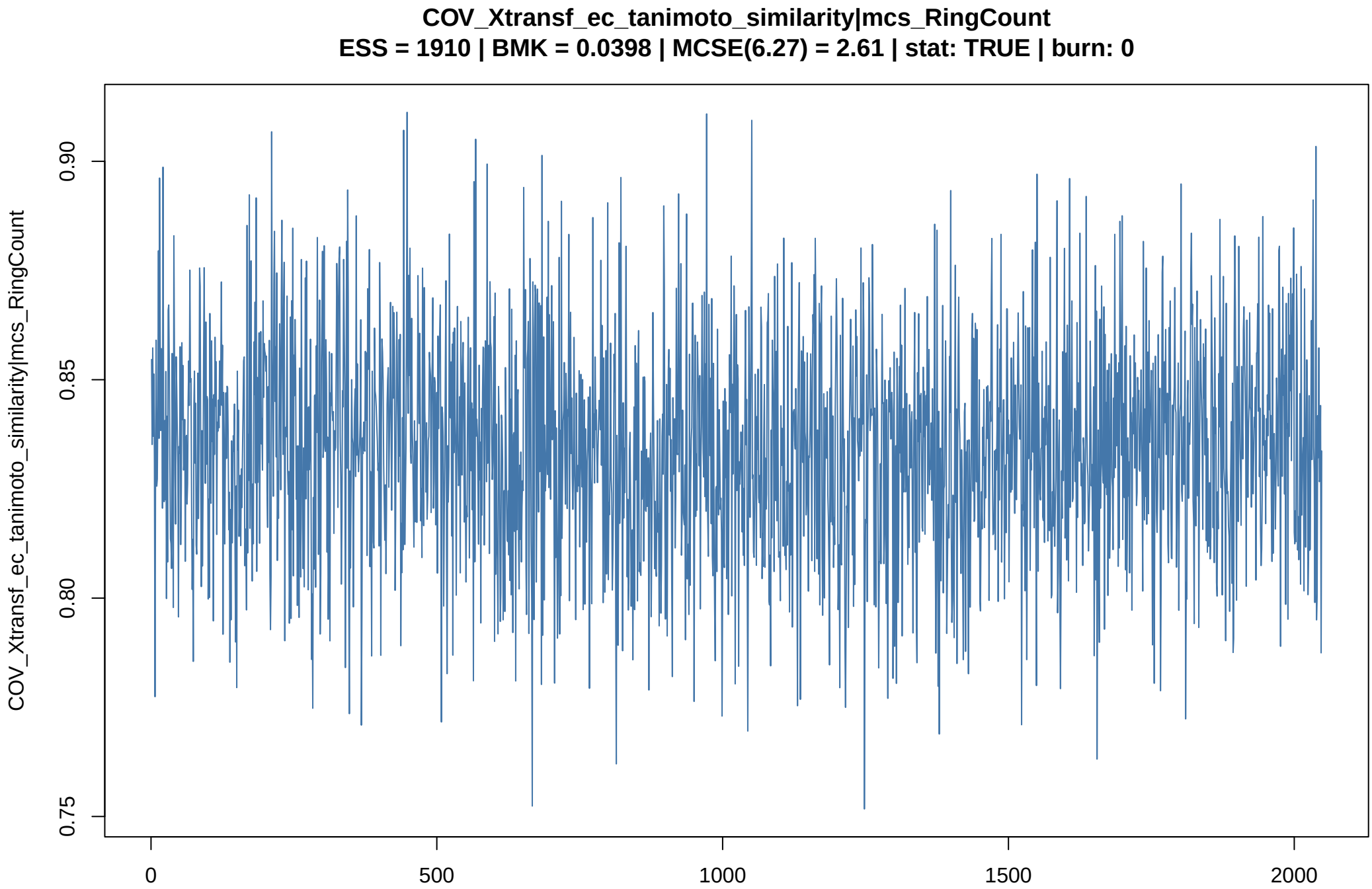

COV_log_RMSD|template_HeavyAtomCount
ESS = 1740 | BMK = 0.044 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.3
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

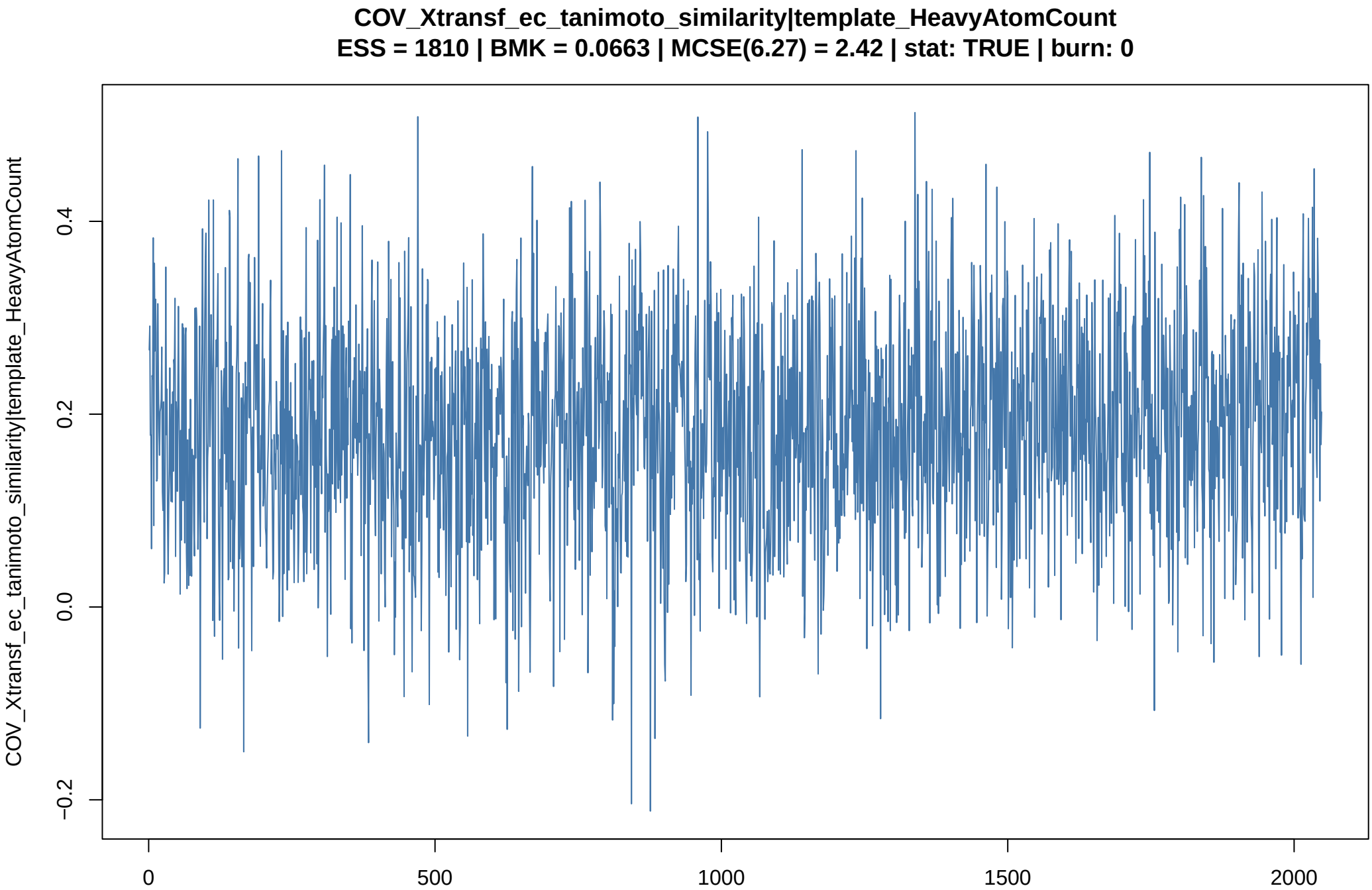

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0414 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

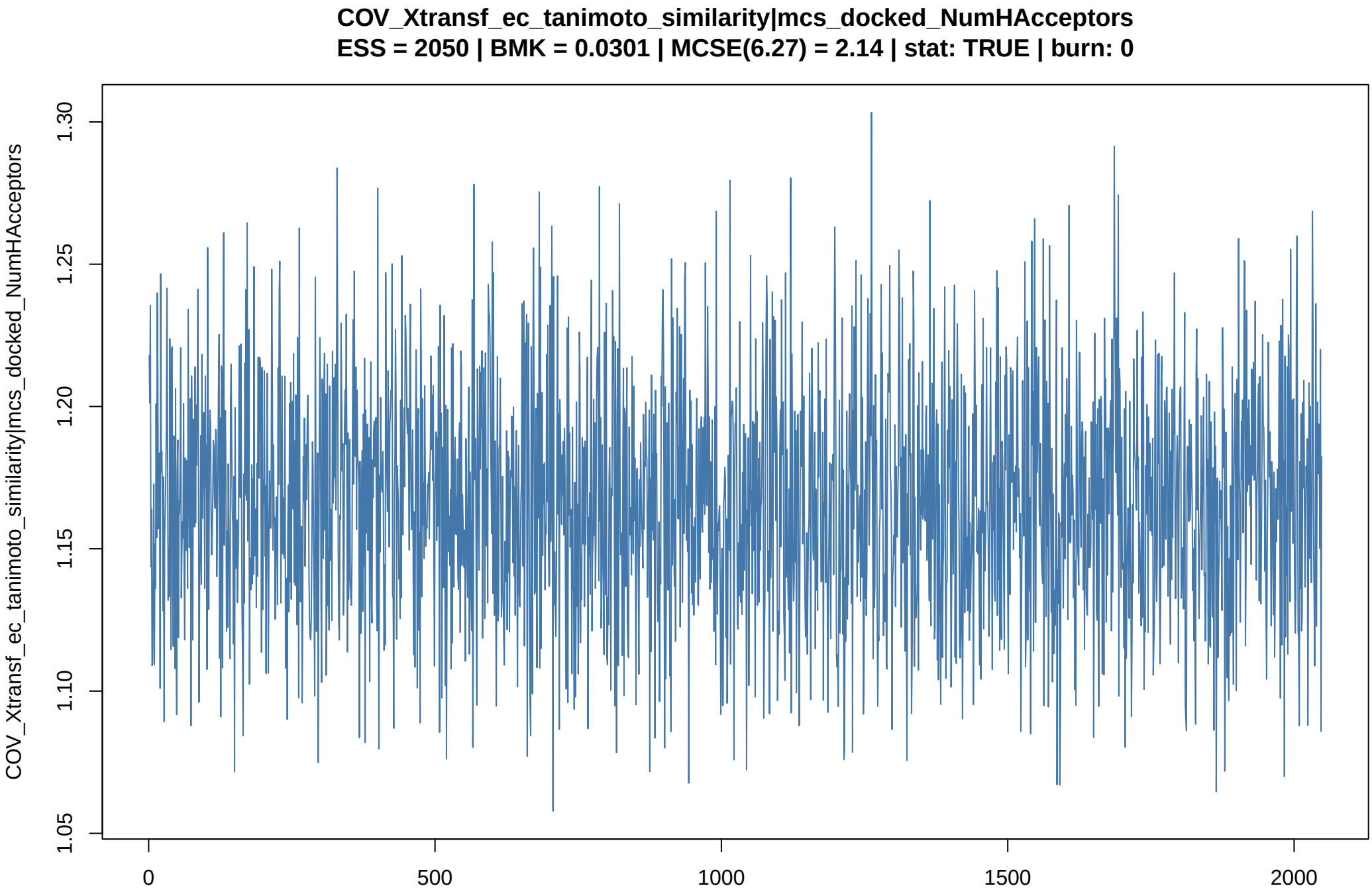

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0322 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

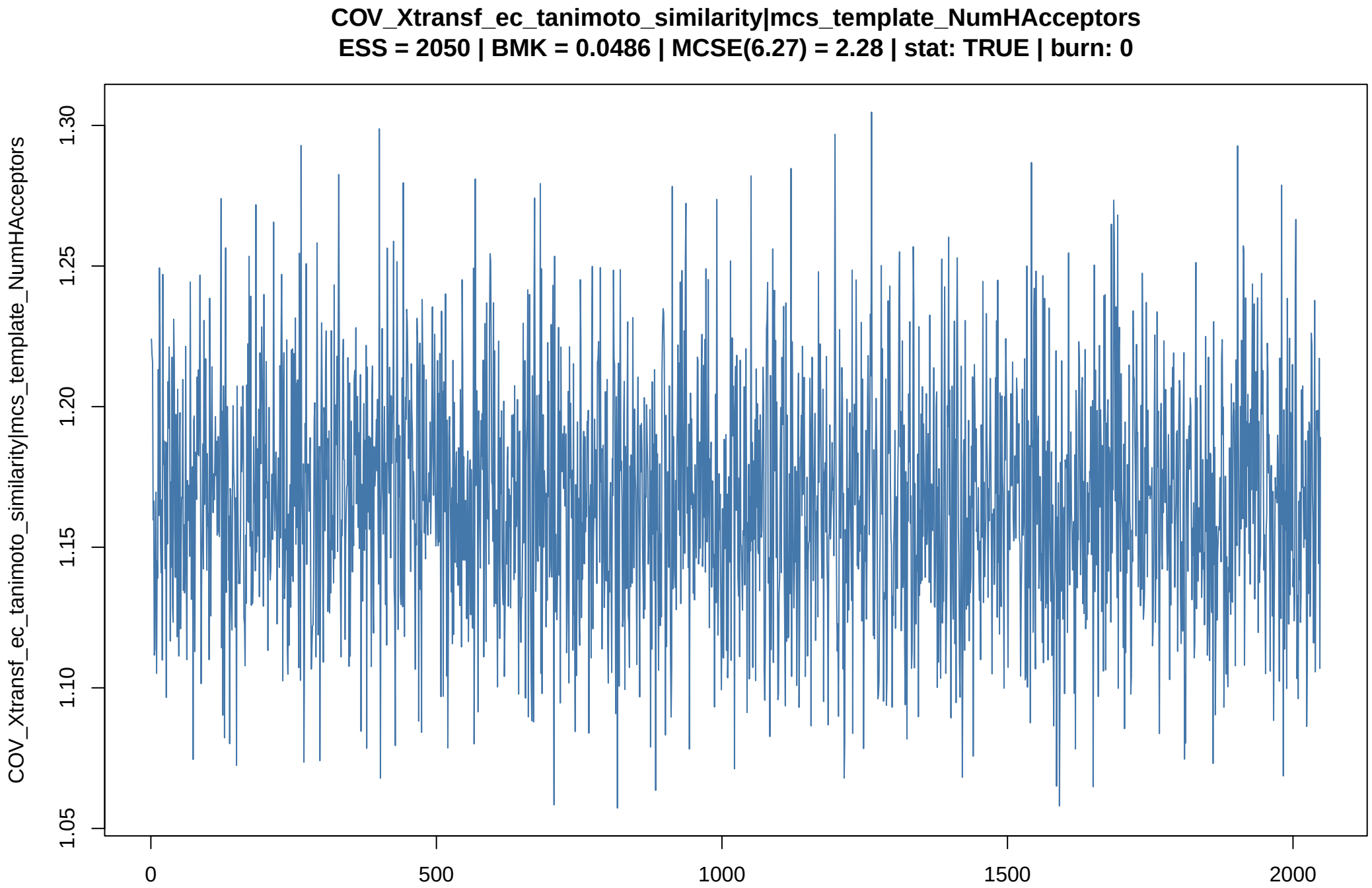

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.65
−0.70
0
500
1000
1500
2000

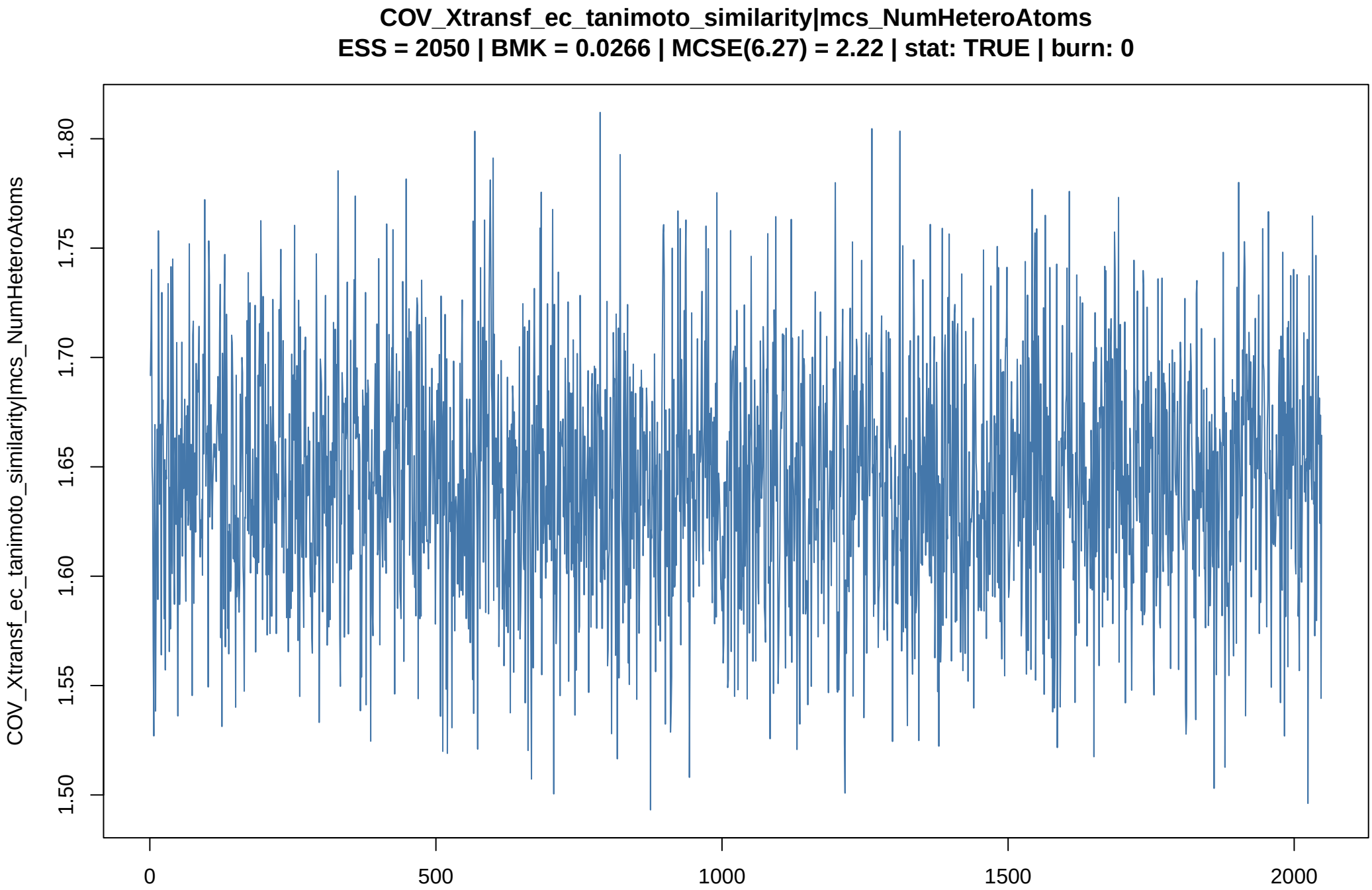

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1870 | BMK = 0.0506 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

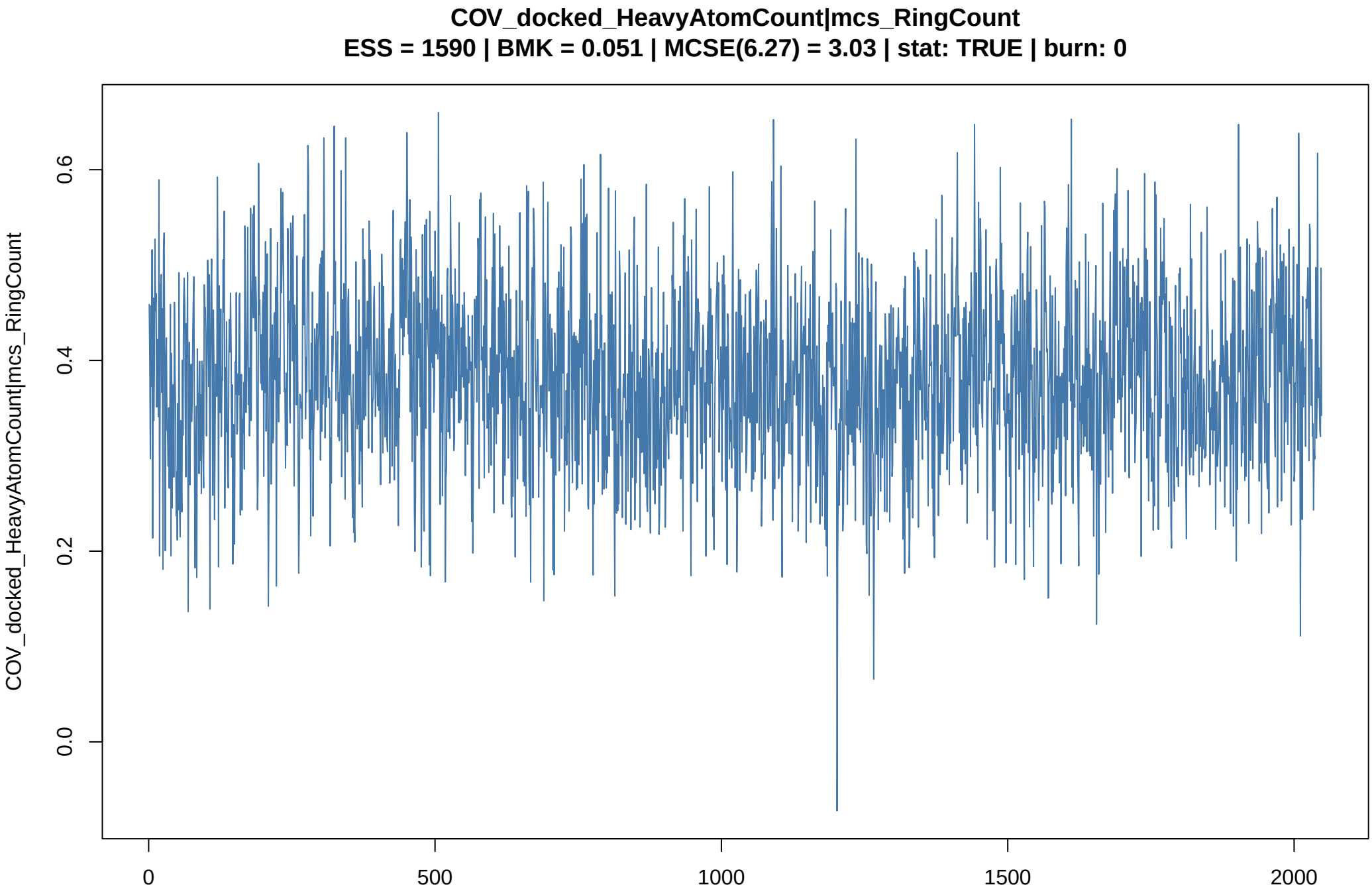

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1910 | BMK = 0.0398 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

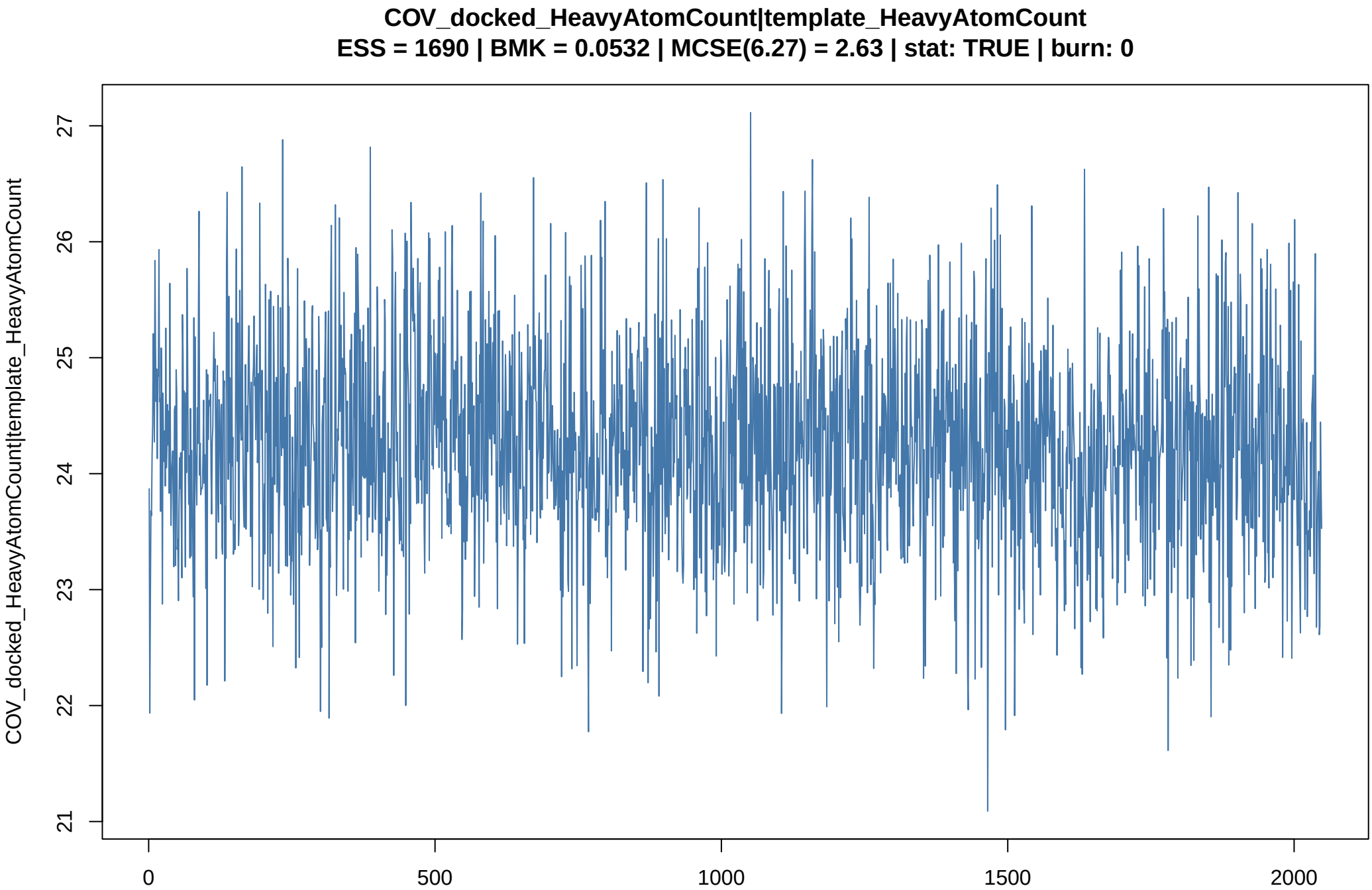

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1810 | BMK = 0.0663 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
−0.2
0.0
0.2
0.4
0
500
1000
1500
2000

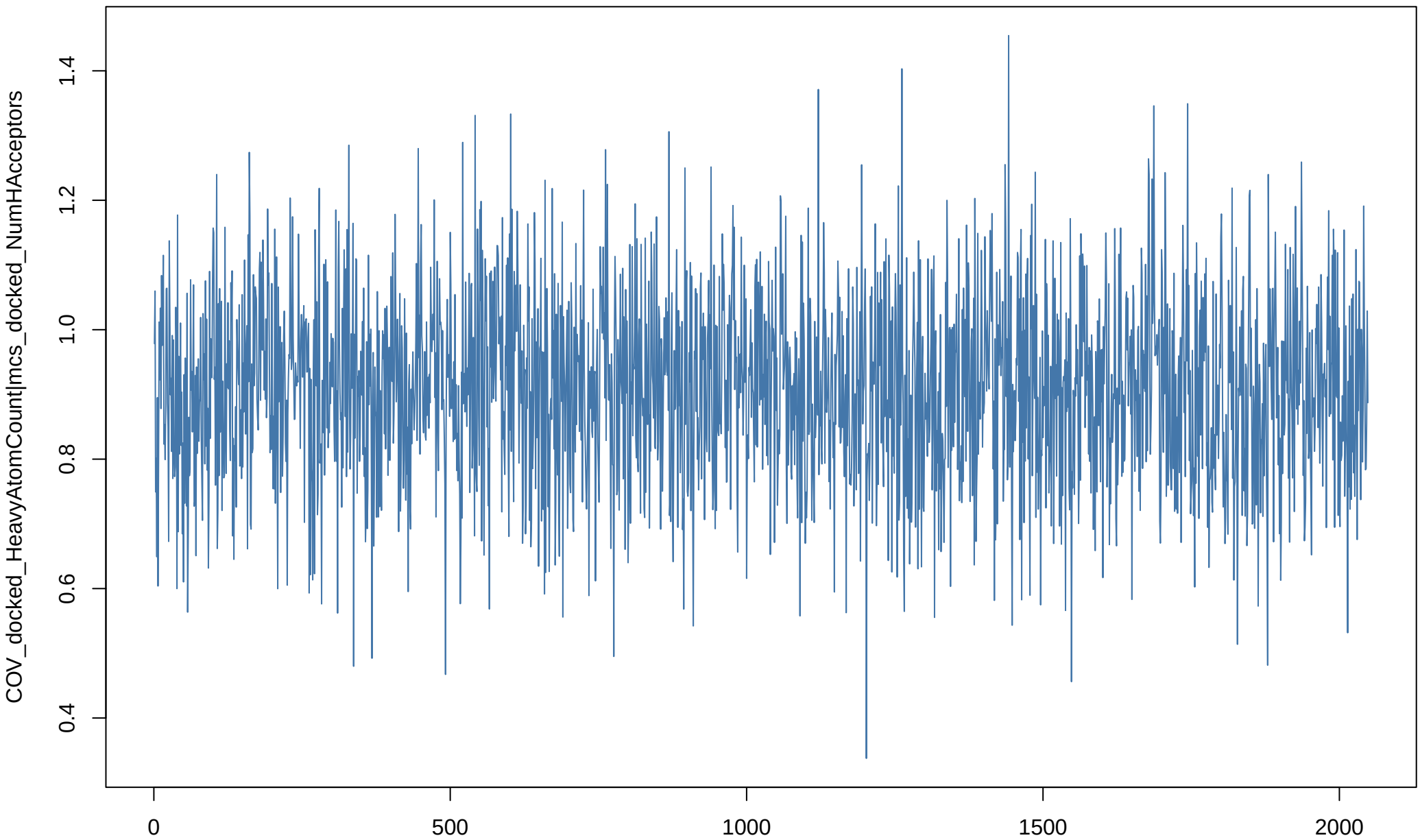

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0301 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

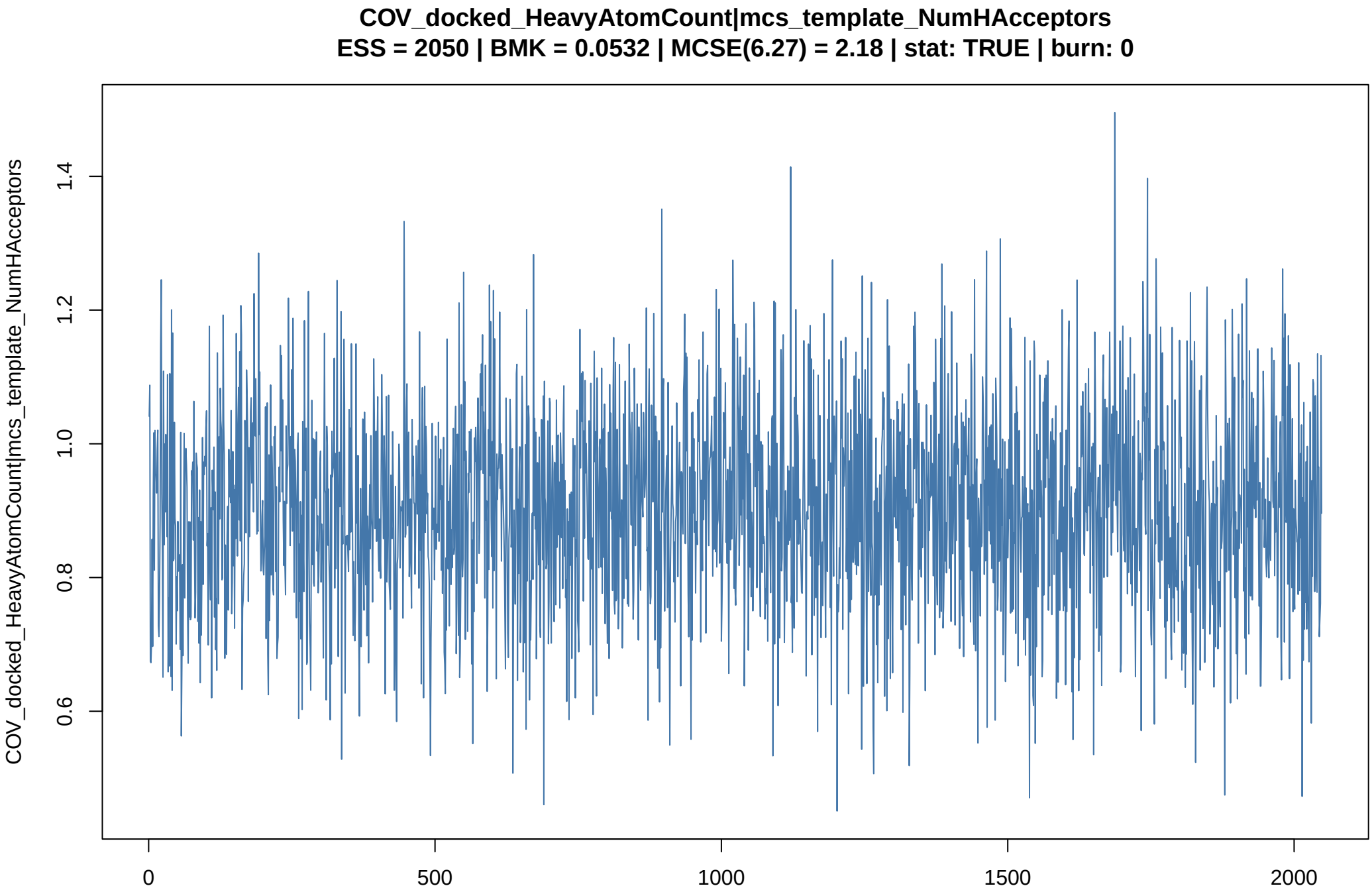

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0486 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

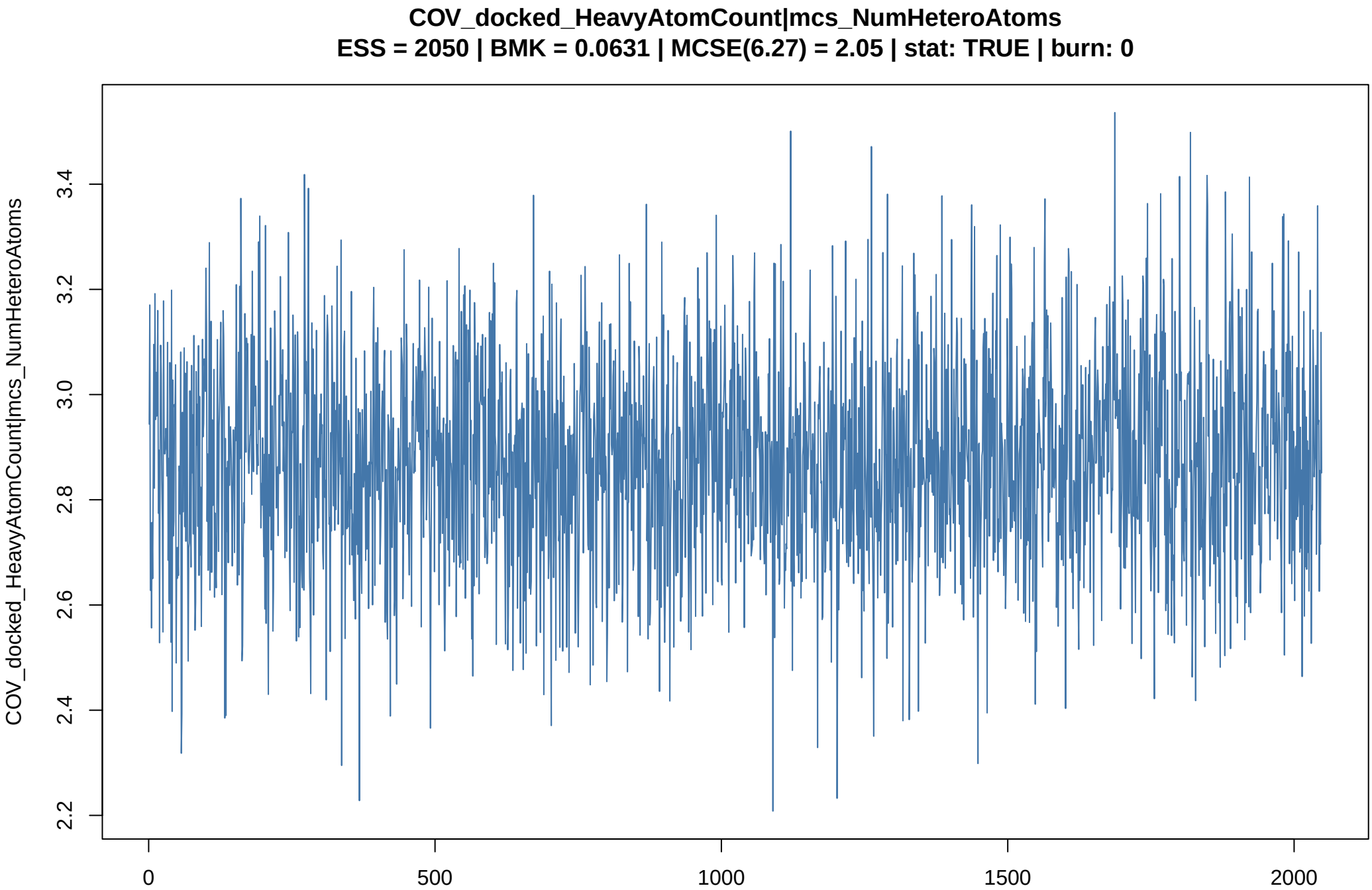

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0266 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.50
1.55
1.60
1.65
1.70
1.75
1.80
0
500
1000
1500
2000

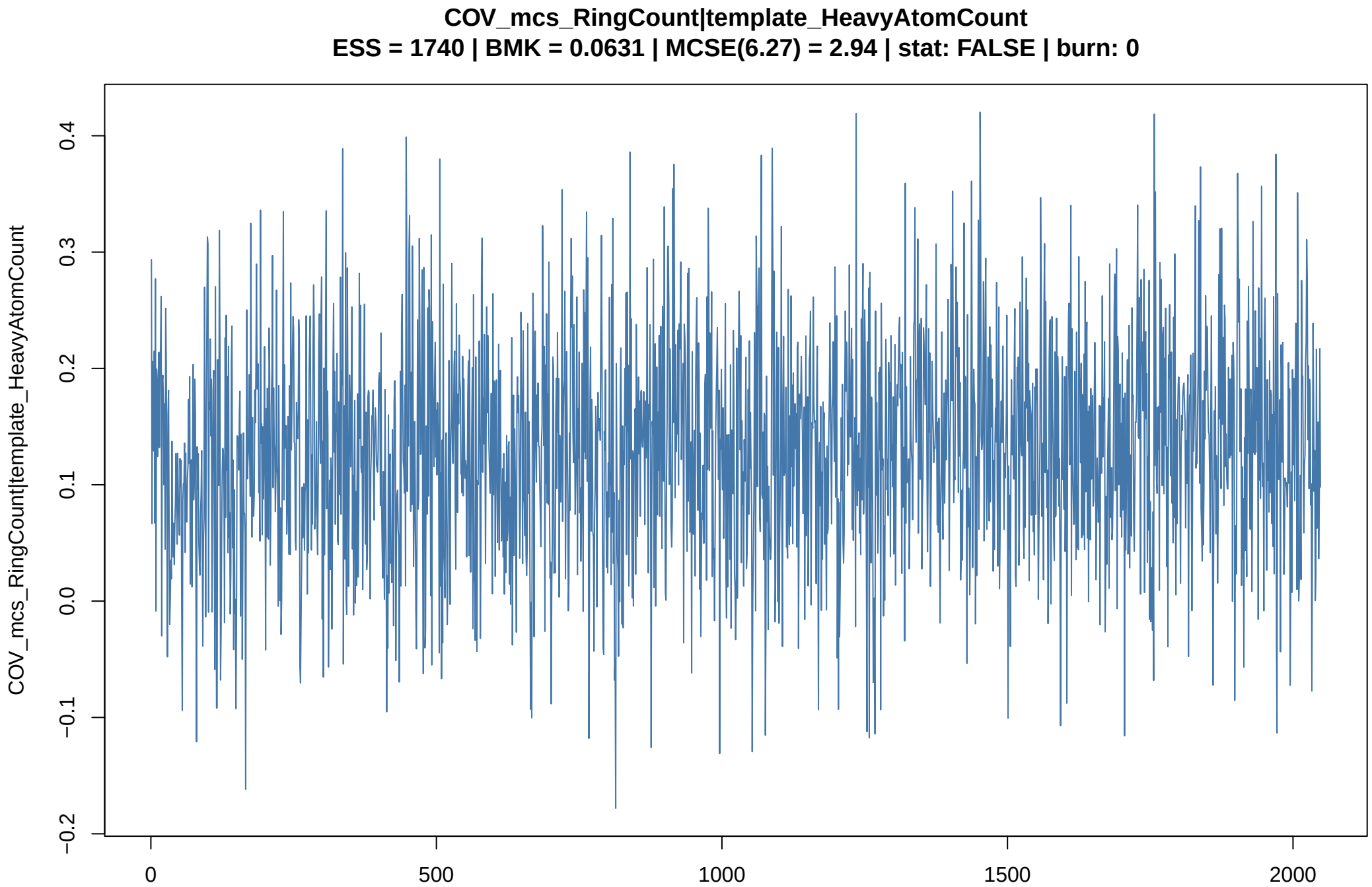

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1590 | BMK = 0.051 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
0.2
0.4
0.6
0
500
1000
1500
2000

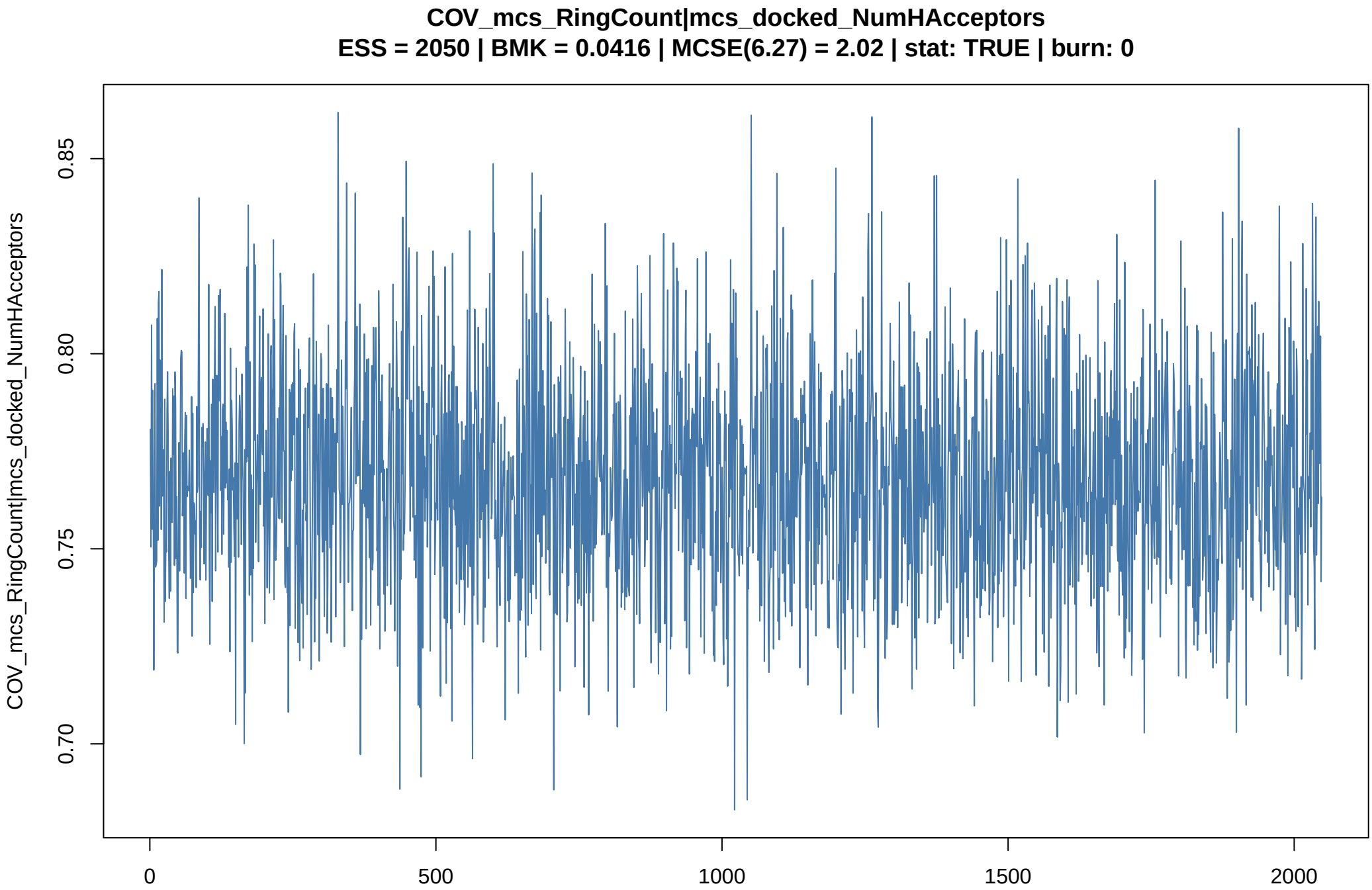

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1690 | BMK = 0.0532 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
21
22
23
24
25
26
27
0
500
1000
1500
2000

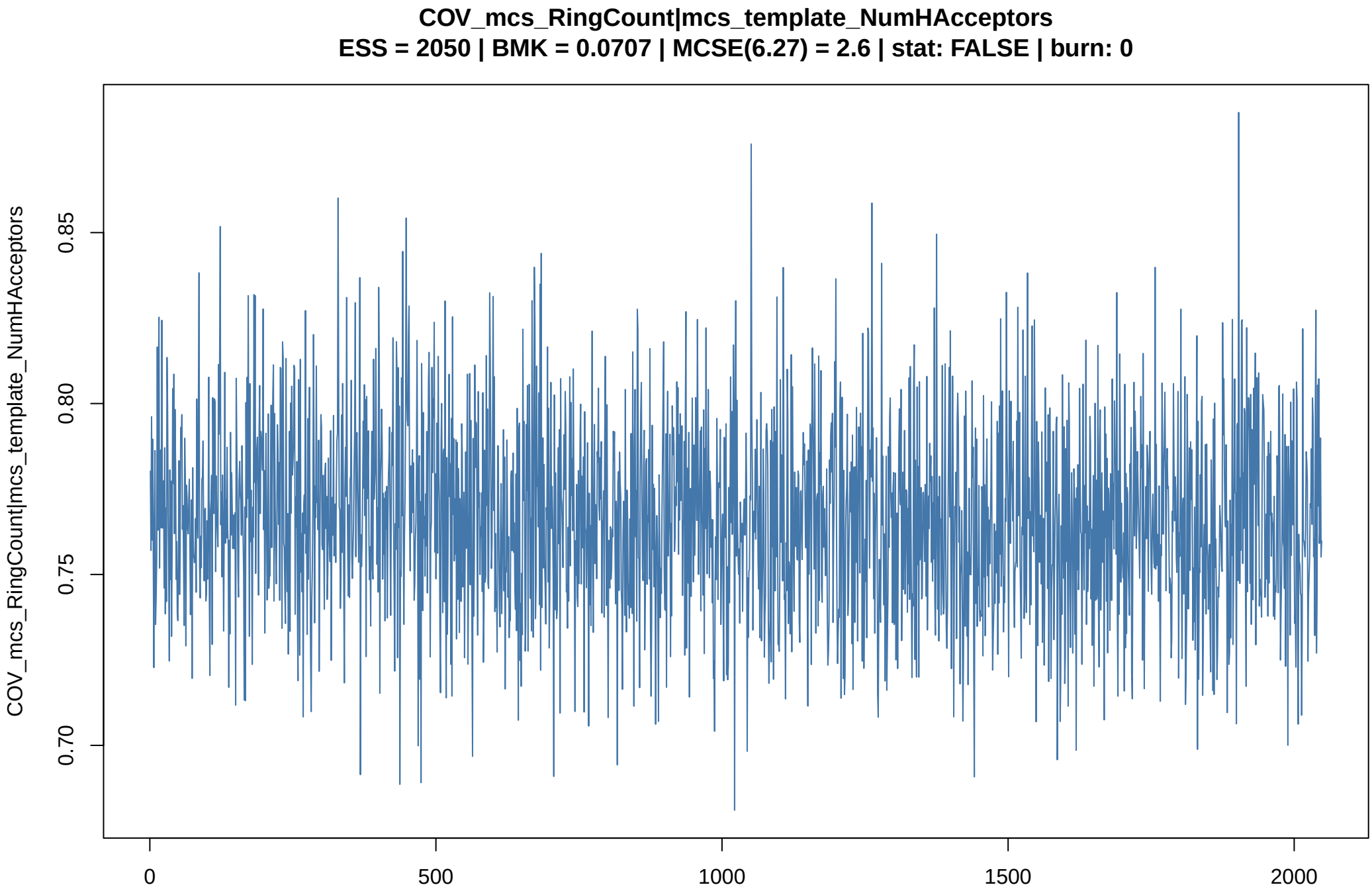

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0472 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

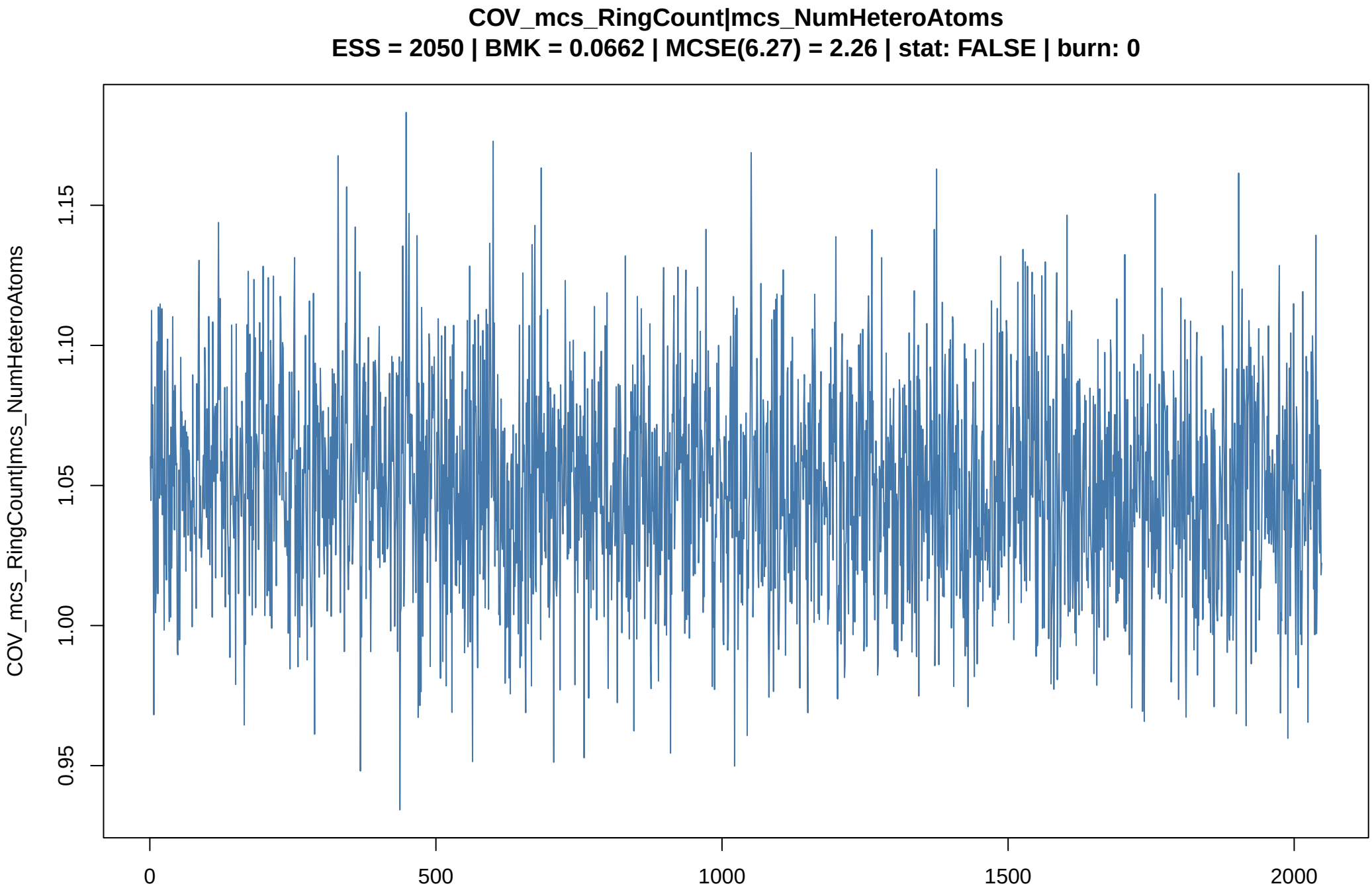

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0532 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

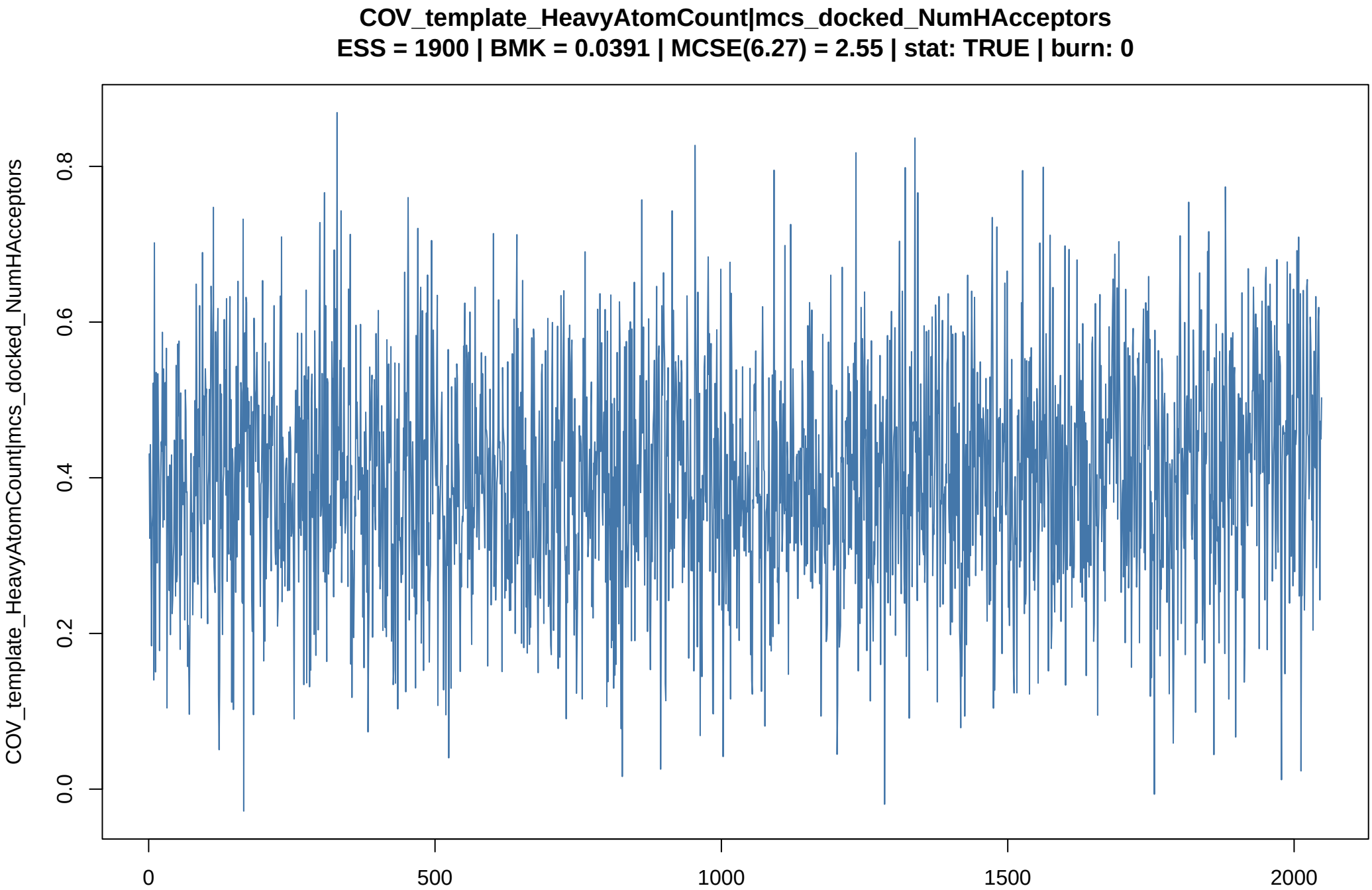

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0631 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
3.2
3.4
0
500
1000
1500
2000

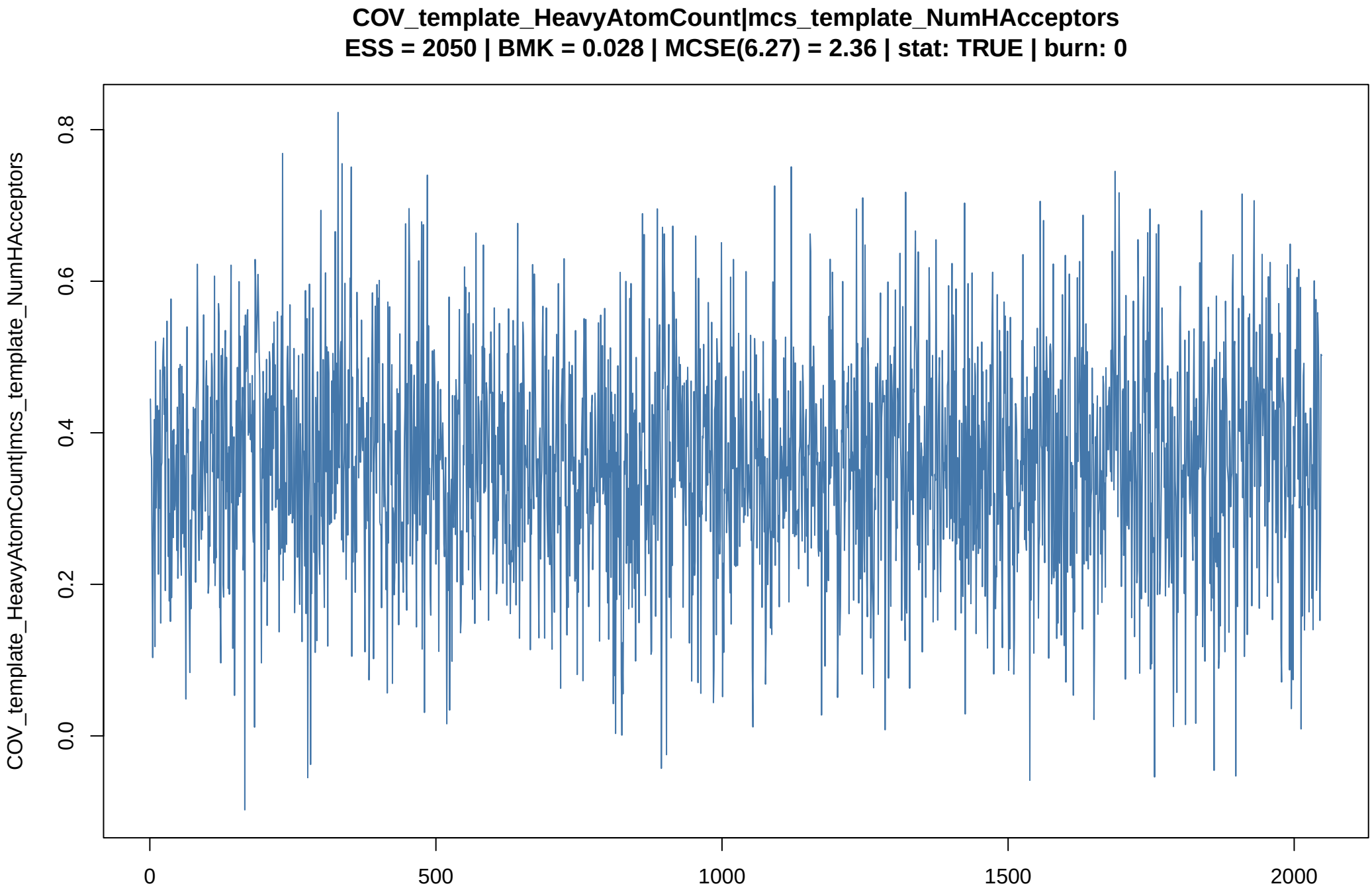

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1740 | BMK = 0.0631 | MCSE(6.27) = 2.94 | stat: FALSE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

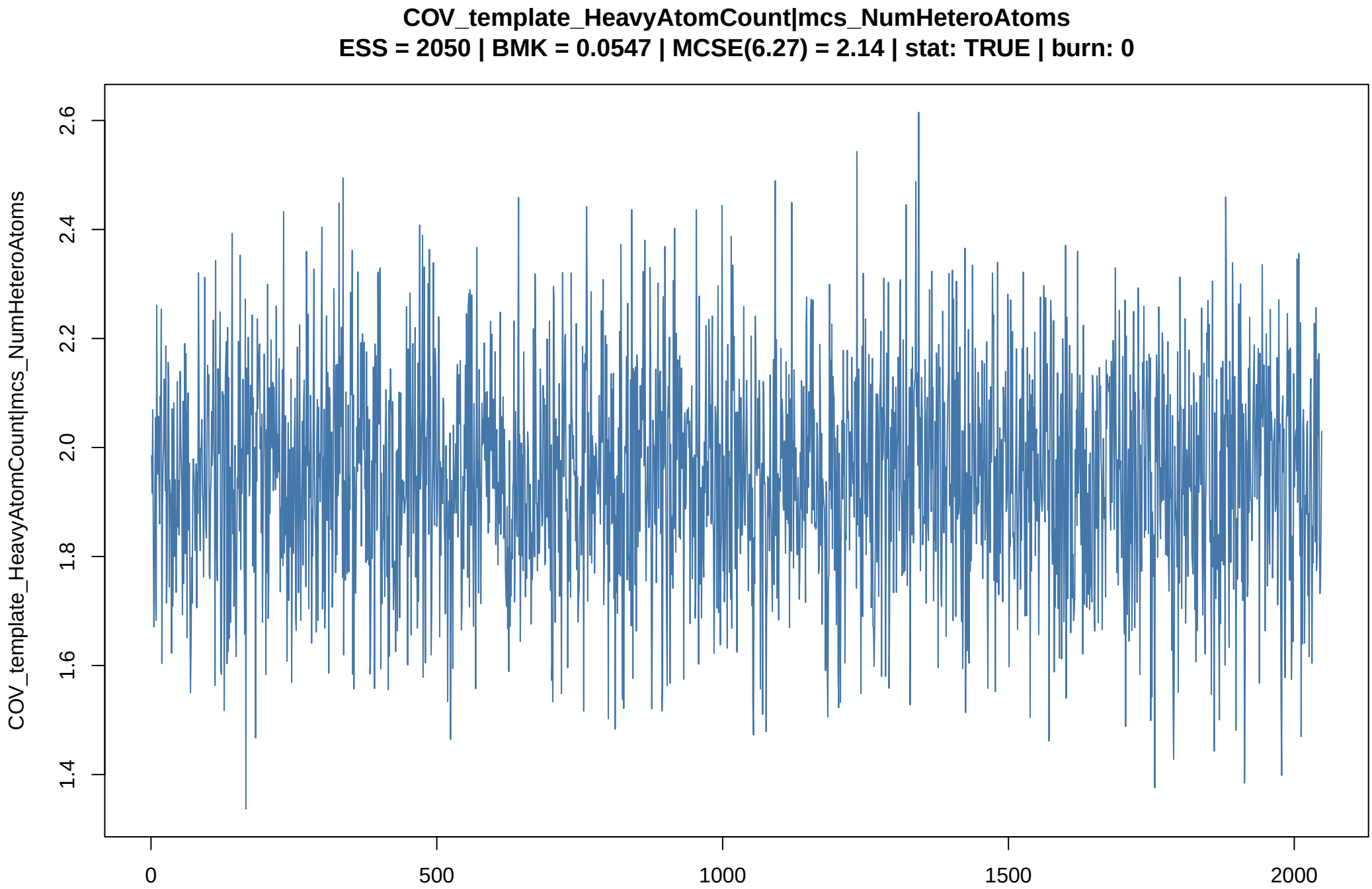

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0416 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

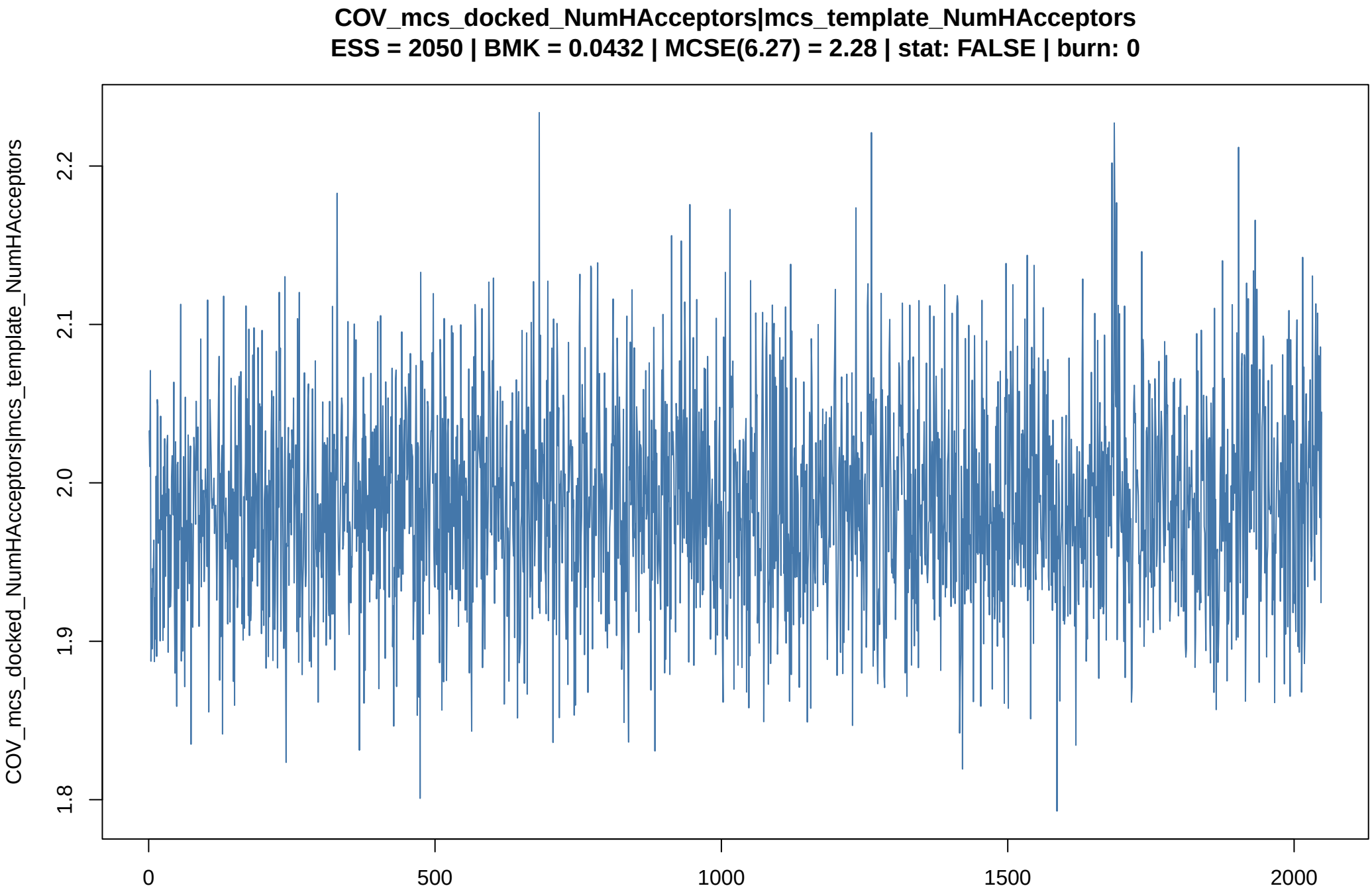

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0707 | MCSE(6.27) = 2.6 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

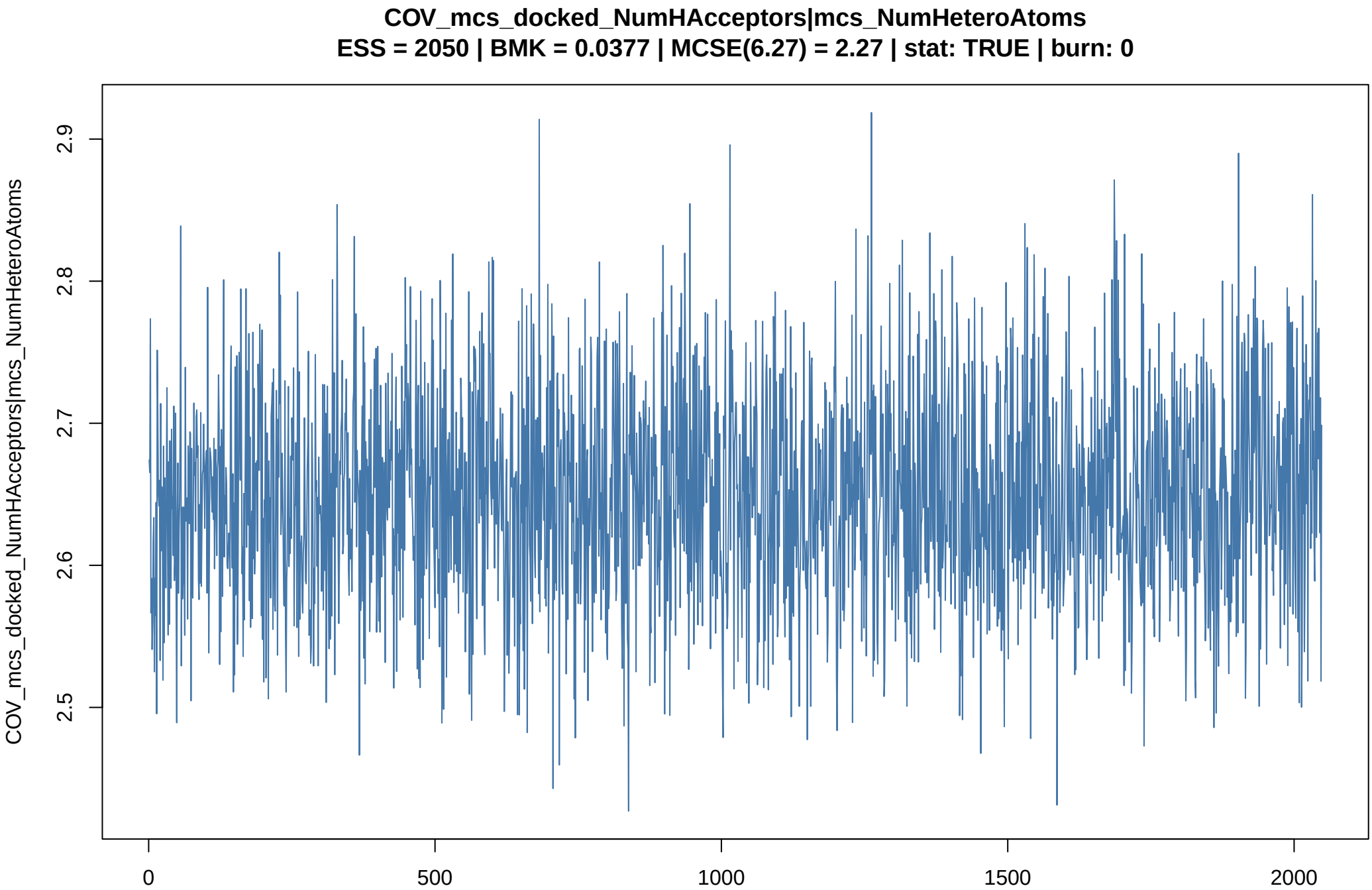

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0662 | MCSE(6.27) = 2.26 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
0
500
1000
1500
2000

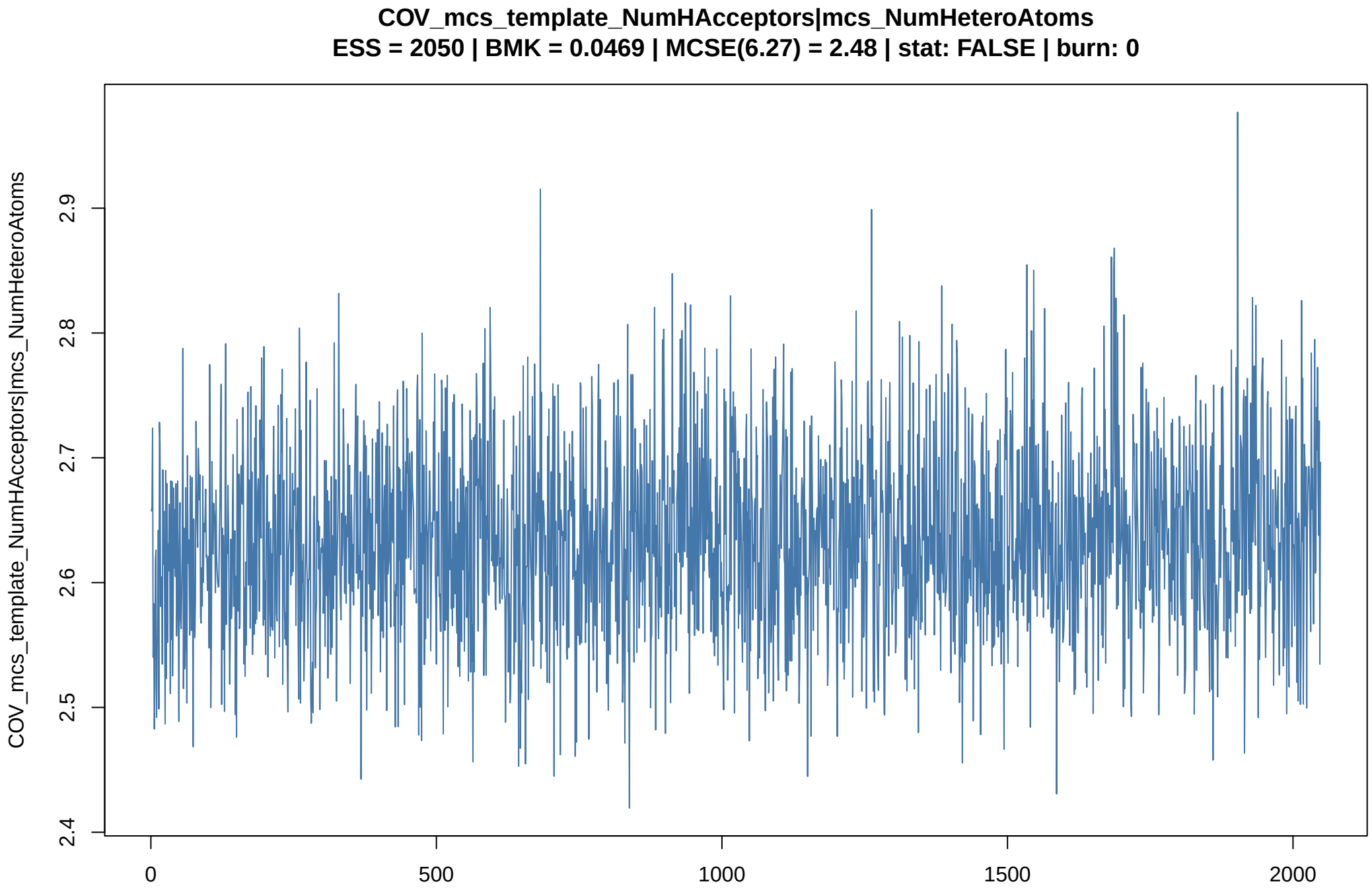

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1900 | BMK = 0.0391 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.028 | MCSE(6.27) = 2.36 | 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 = 2050 | BMK = 0.0547 | MCSE(6.27) = 2.14 | 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 = 0.0432 | MCSE(6.27) = 2.28 | stat: FALSE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0377 | MCSE(6.27) = 2.27 | 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 = 0.0469 | MCSE(6.27) = 2.48 | 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