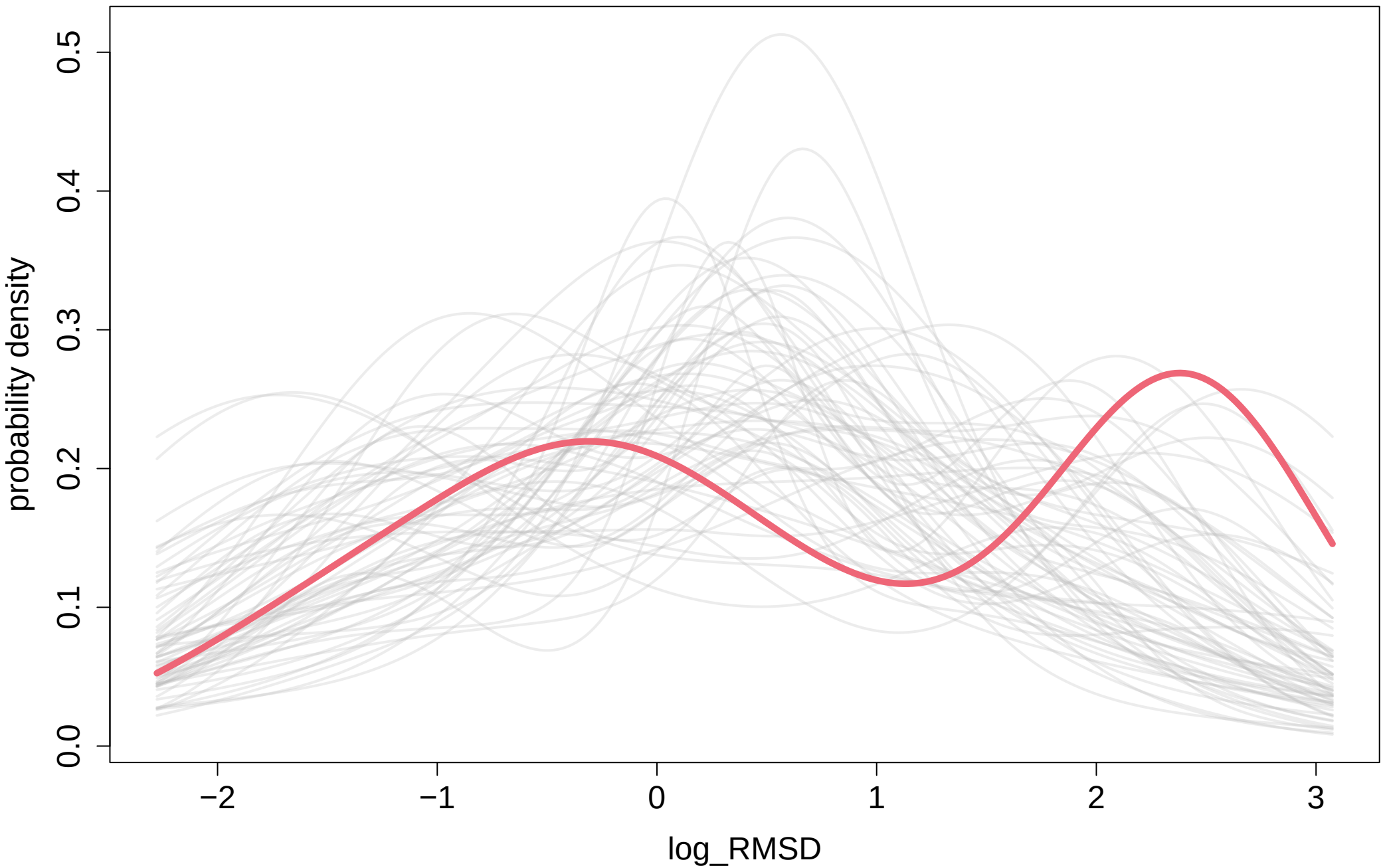
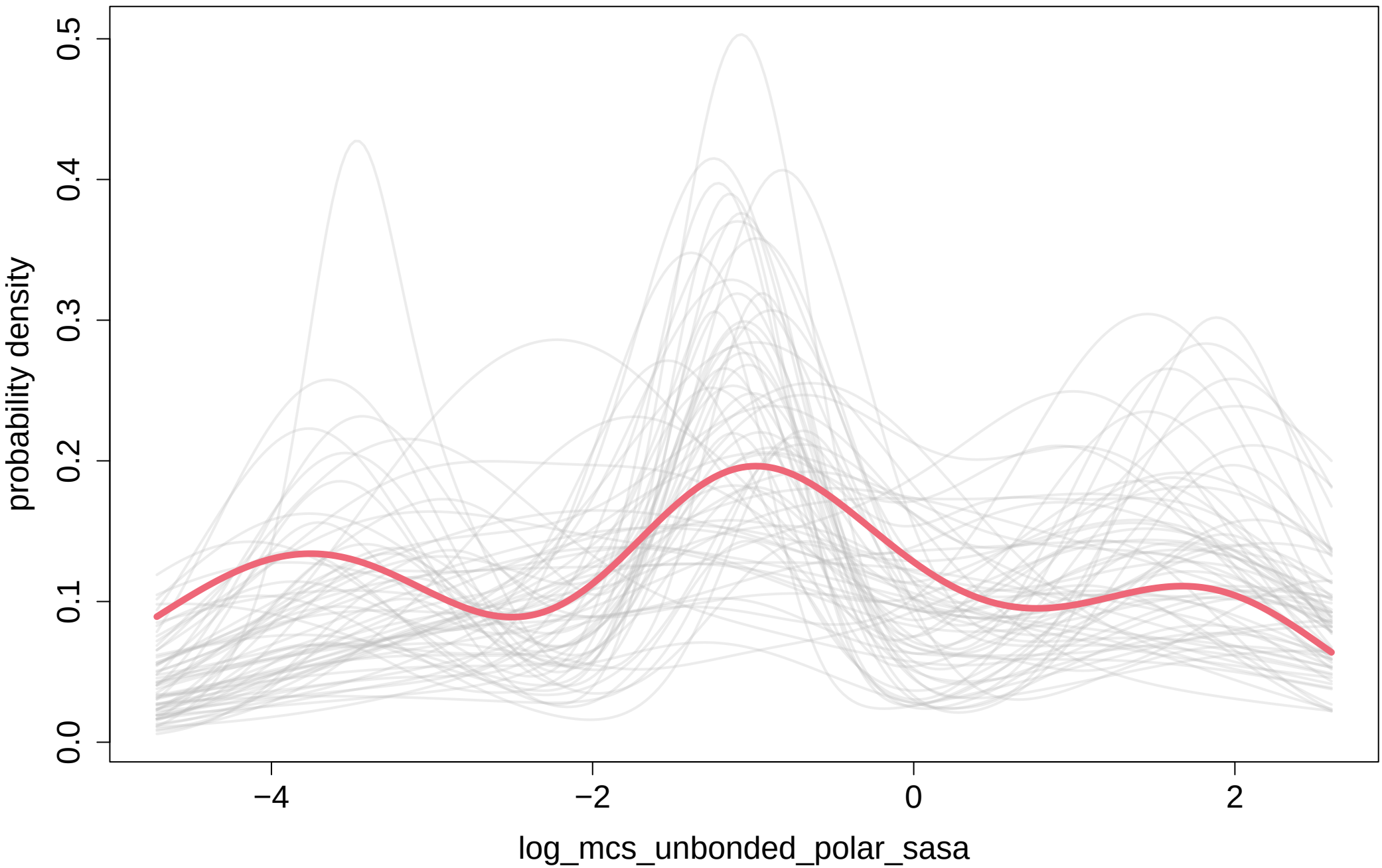
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = 18.3243242311238
all stationary: FALSE
burn: 100
min percent.: 2

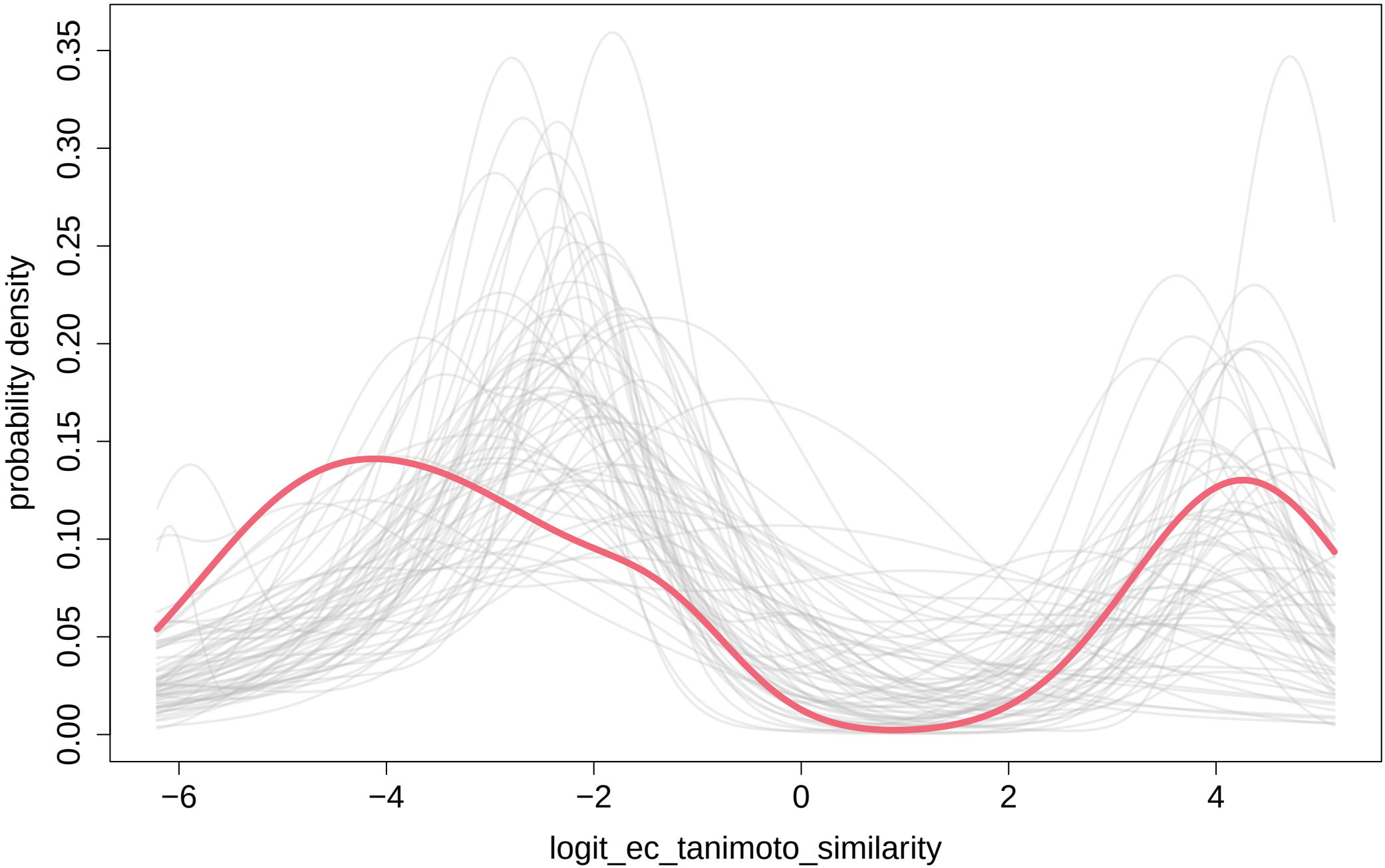
−− STATS 2D −−
min ESS = 17.6868794487031
max BMK = 0.375515787624467
max MCSE = 26.7607691234983
all stationary: FALSE
burn: 100
min percent.: 1

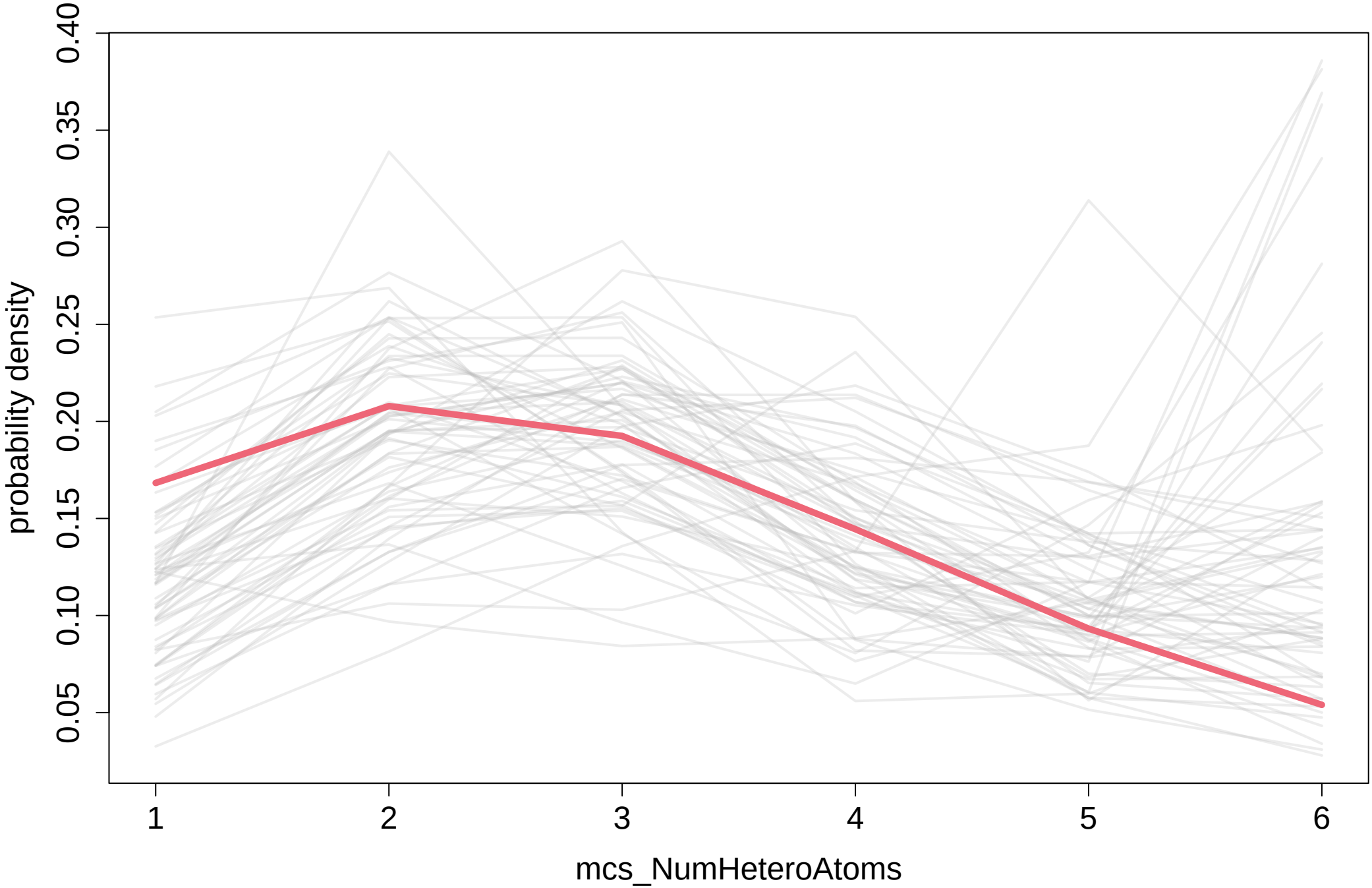
−− STATS 1D −−
min ESS = 20.2737133632079
max BMK = 1
max MCSE = 29.6487864032052
all stationary: FALSE
burn: 100
min percent.: 0

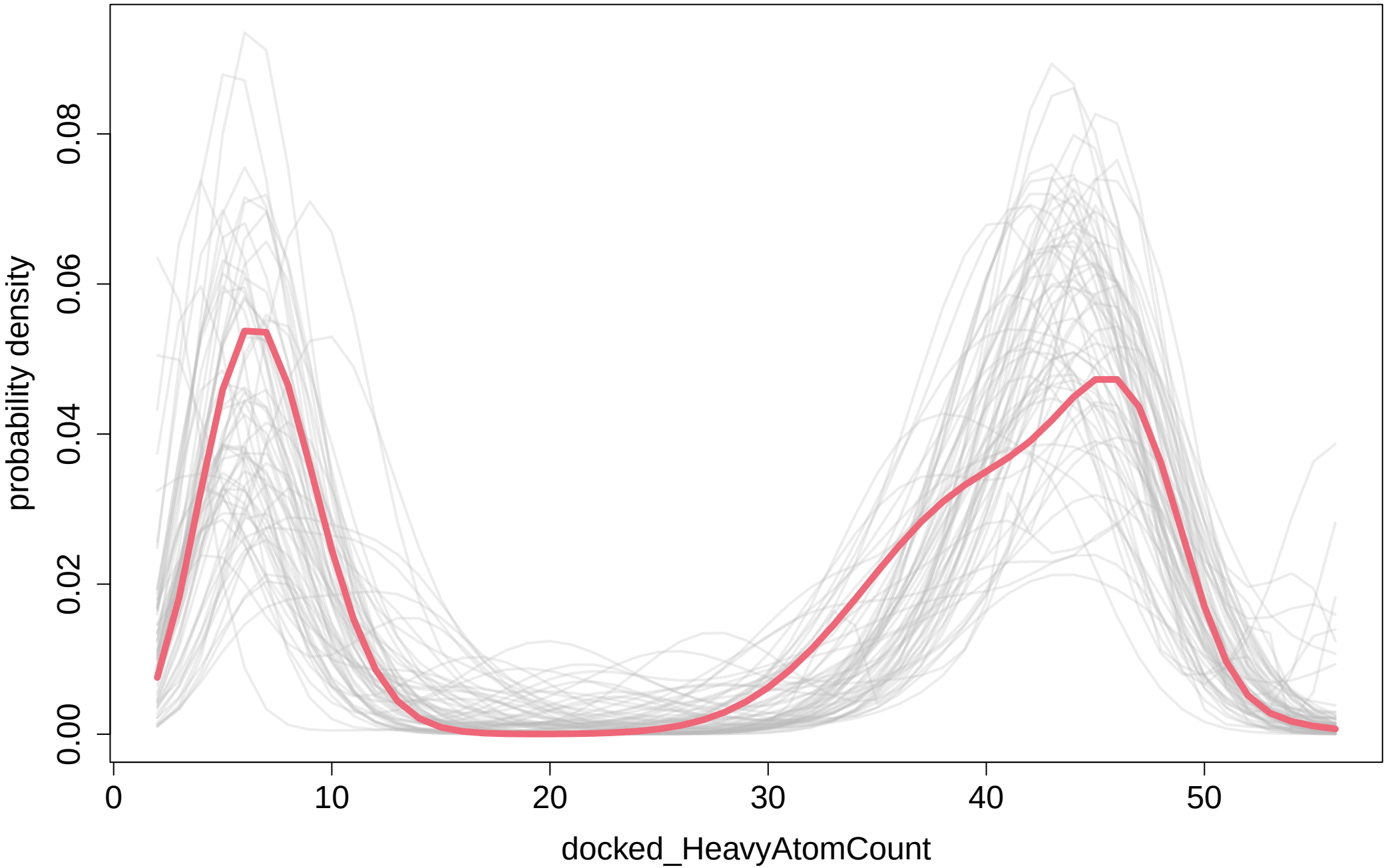
Occupied clusters: 4 of 64
LL: −244 +− 9.56


probability density
0.0
0.1
0.2
0.3
0.4
0.5
−2
−1
0
1
2
3
log_RMSD


probability density
0.0
0.1
0.2
0.3
0.4
0.5
−4
−2
0
2
log_mcs_unbonded_polar_sasa


probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
−6
−4
−2
0
2
4
logit_ec_tanimoto_similarity


probability density
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
1
2
3
4
5
6
mcs_NumHeteroAtoms


probability density
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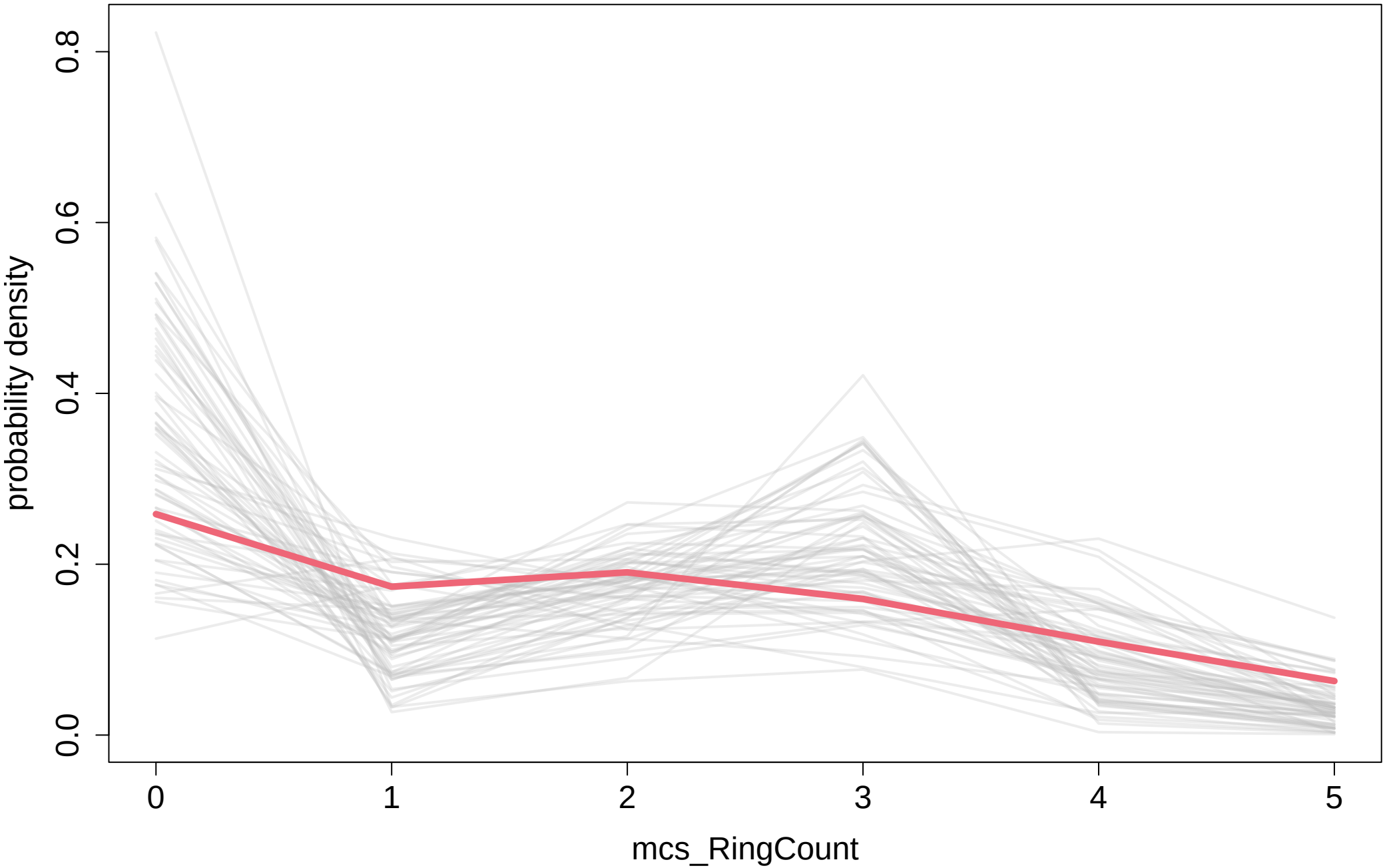
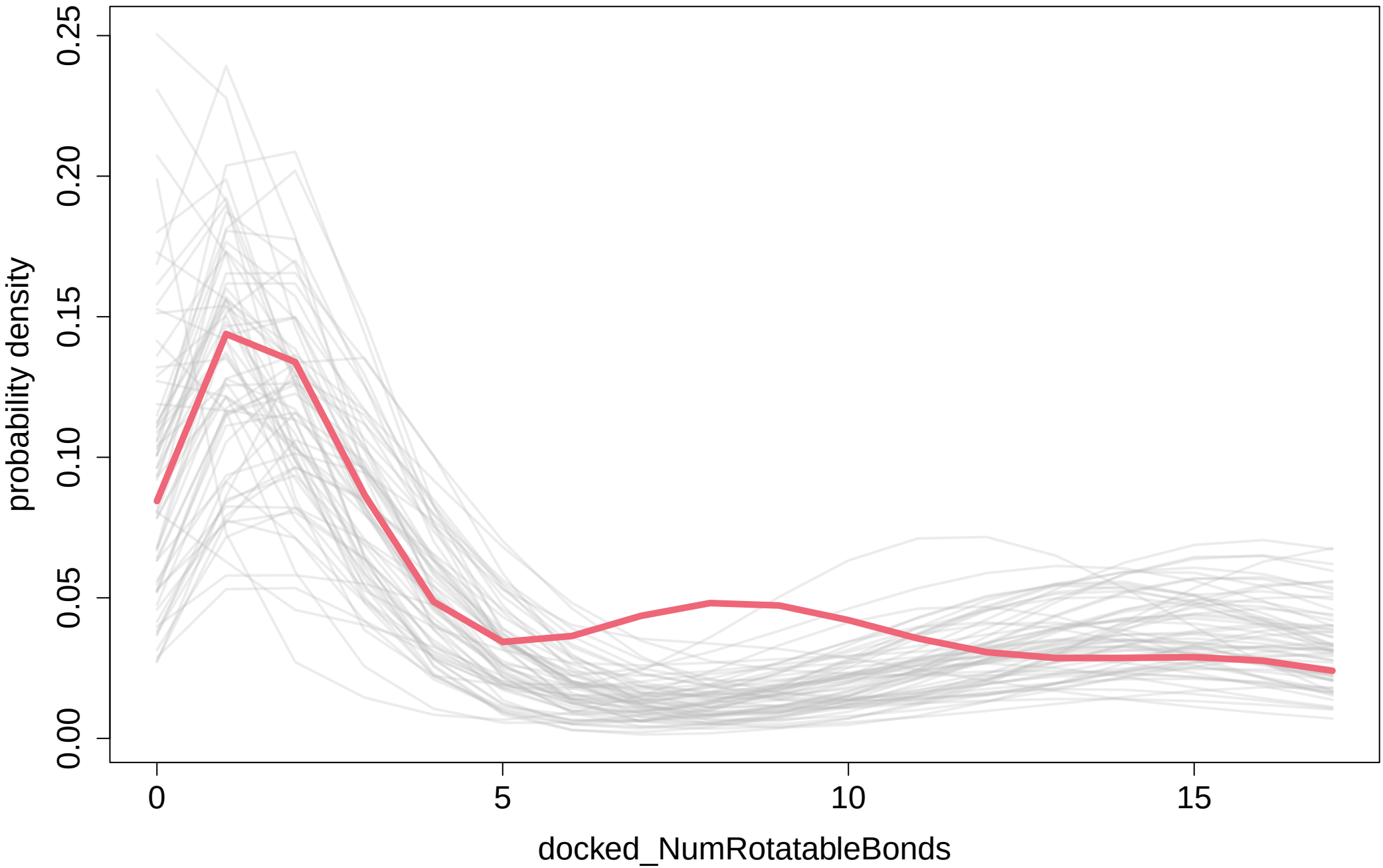
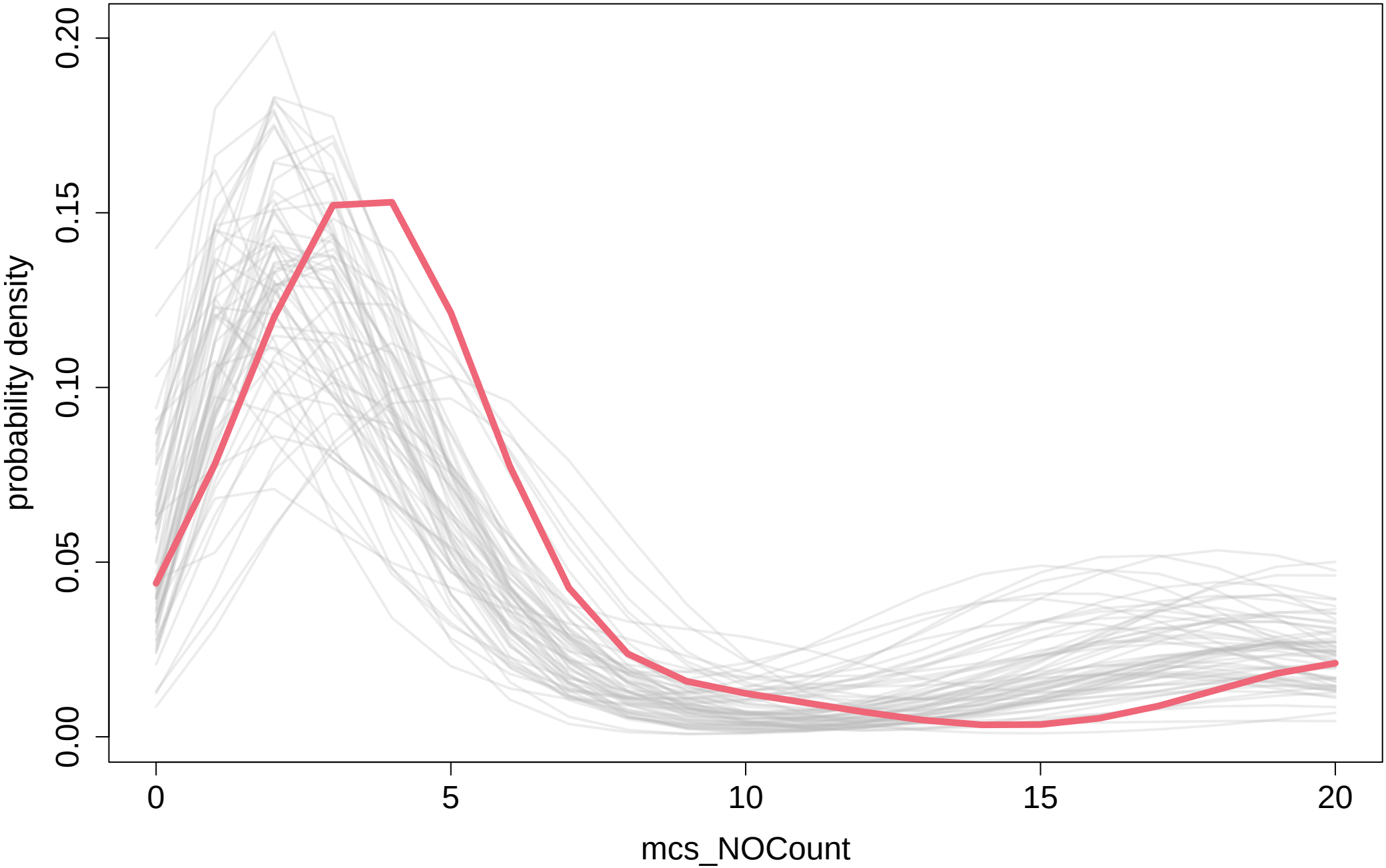
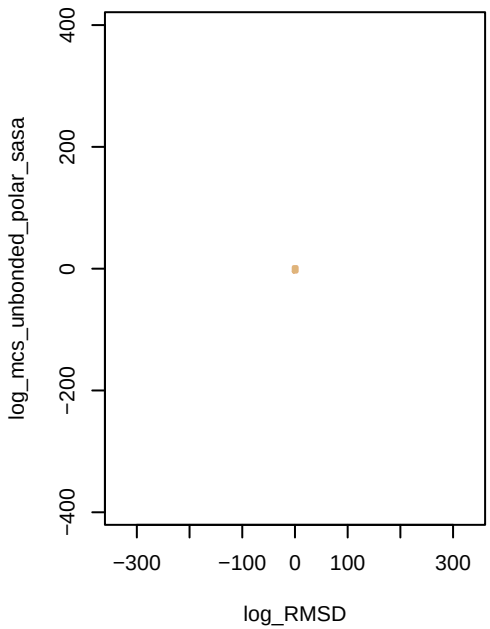
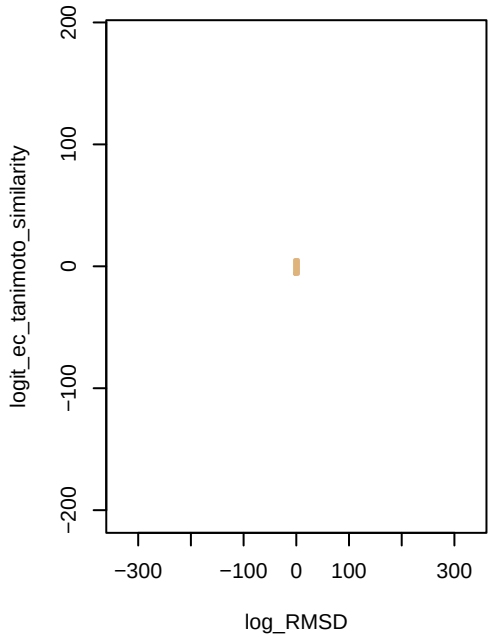
0.02
0.04
0.06
0.08
0
10
20
30
40
50
docked_HeavyAtomCount

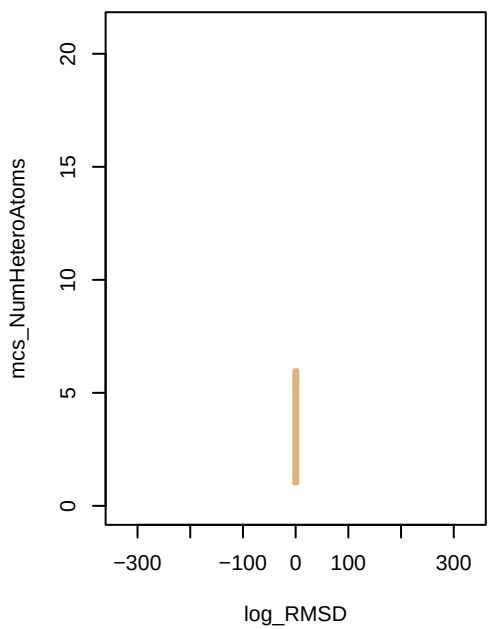

probability density
0.0
0.2
0.4
0.6
0.8
0
1
2
3
4
5
mcs_RingCount

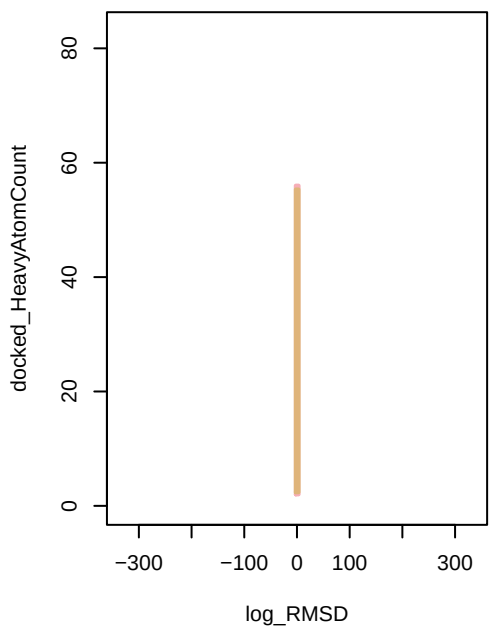

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
docked_NumRotatableBonds

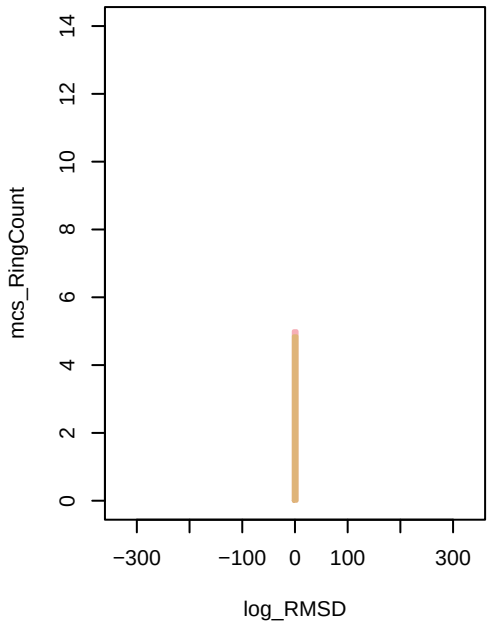

probability density
0.00
0.05
0.10
0.15
0.20
0
5
10
15
20
mcs_NOCount

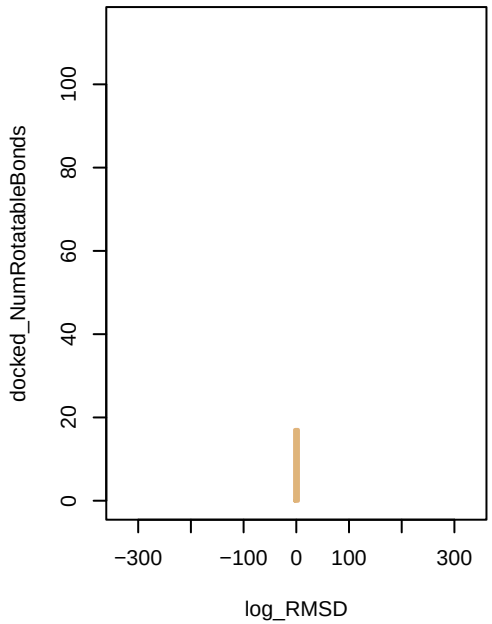

log_mcs_unbonded_polar_sasa
400
200
0
−200
−400
−300
−100
0
100
300
log_RMSD

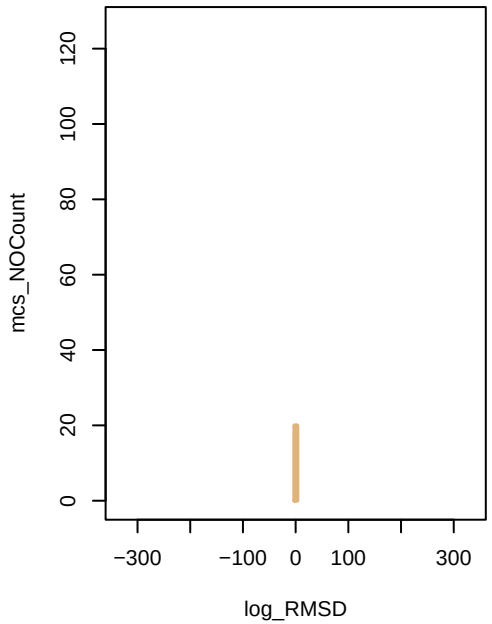

logit_ec_tanimoto_similarity
200
100
0
−100
−200
−300
−100
0
100
300
log_RMSD

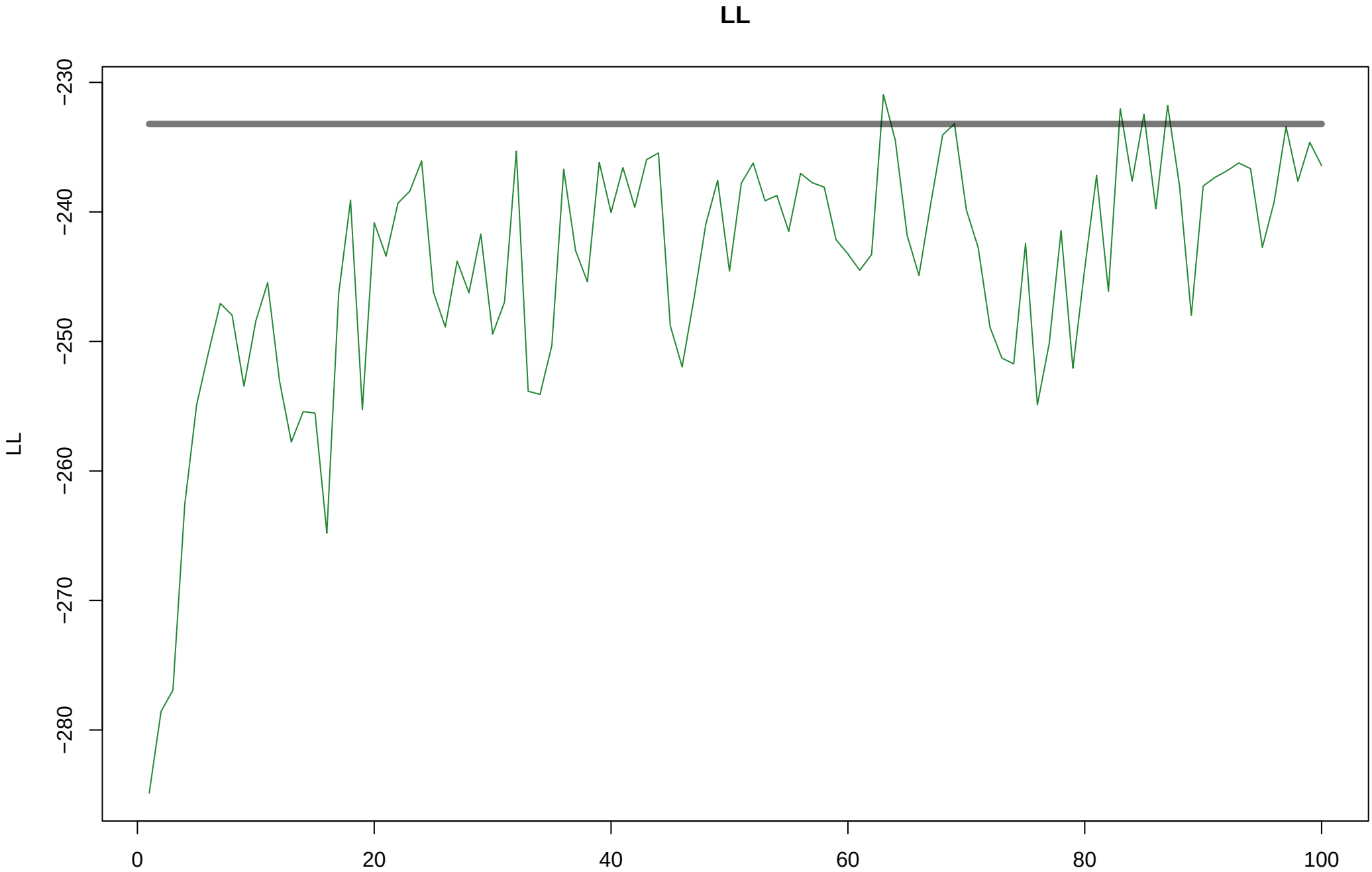

mcs_NumHeteroAtoms
20
15
10
5
0
−300
−100
0
100
300
log_RMSD

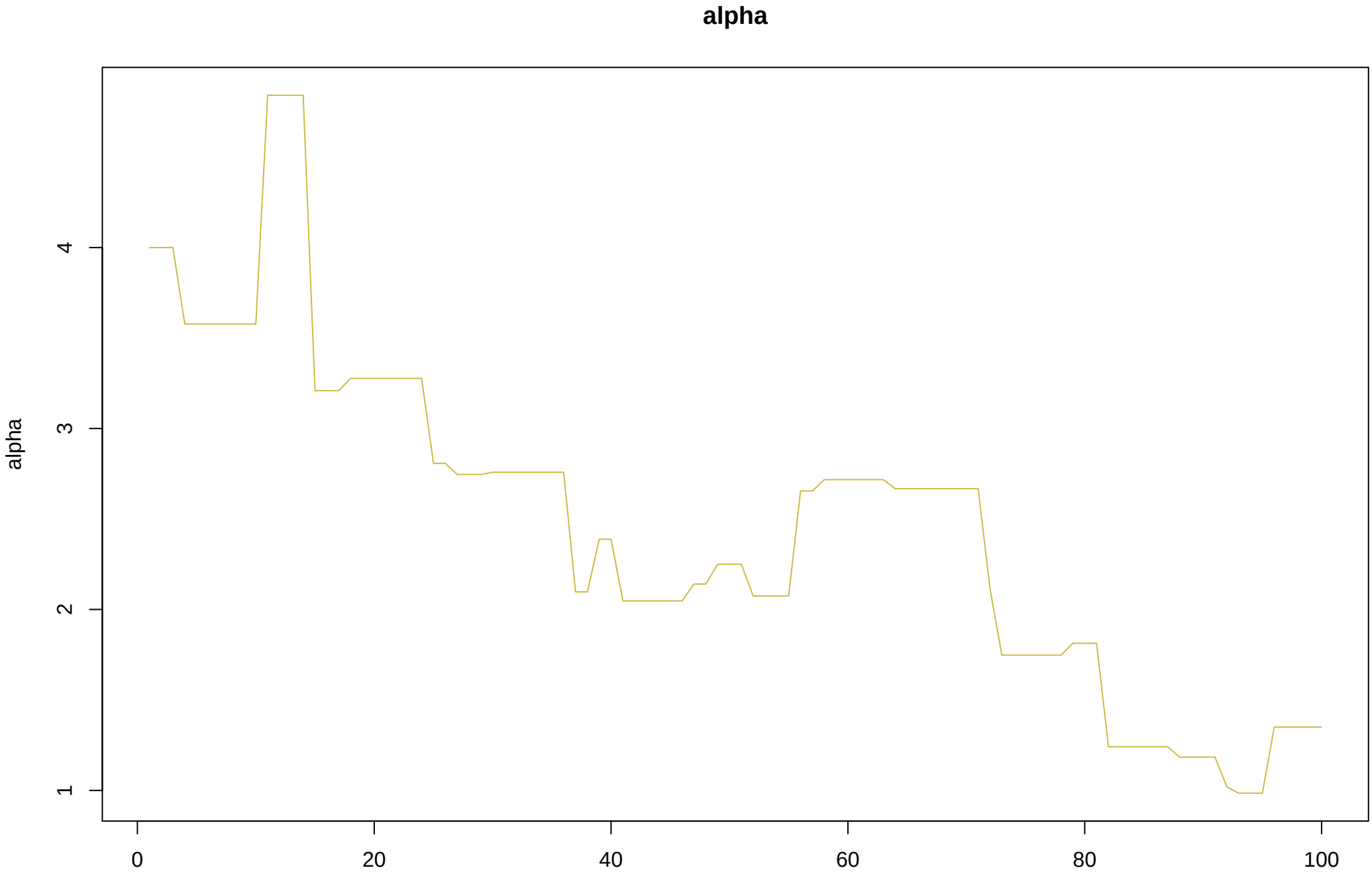

docked_HeavyAtomCount
80
60
40
20
0
−300
−100
0
100
300
log_RMSD

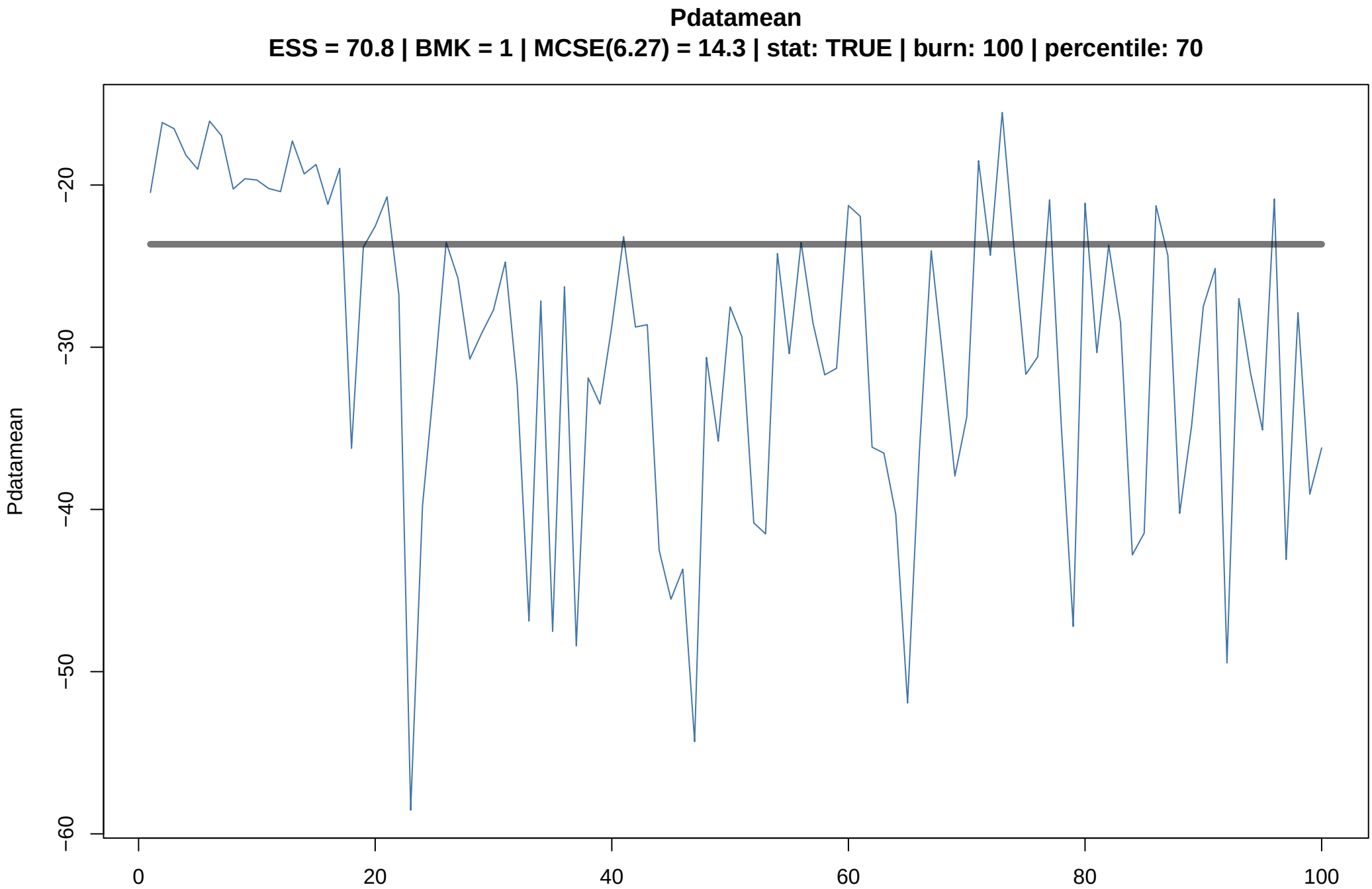

mcs_RingCount
14
12
10
8
6
4
2
0
−300
−100
0
100
300
log_RMSD

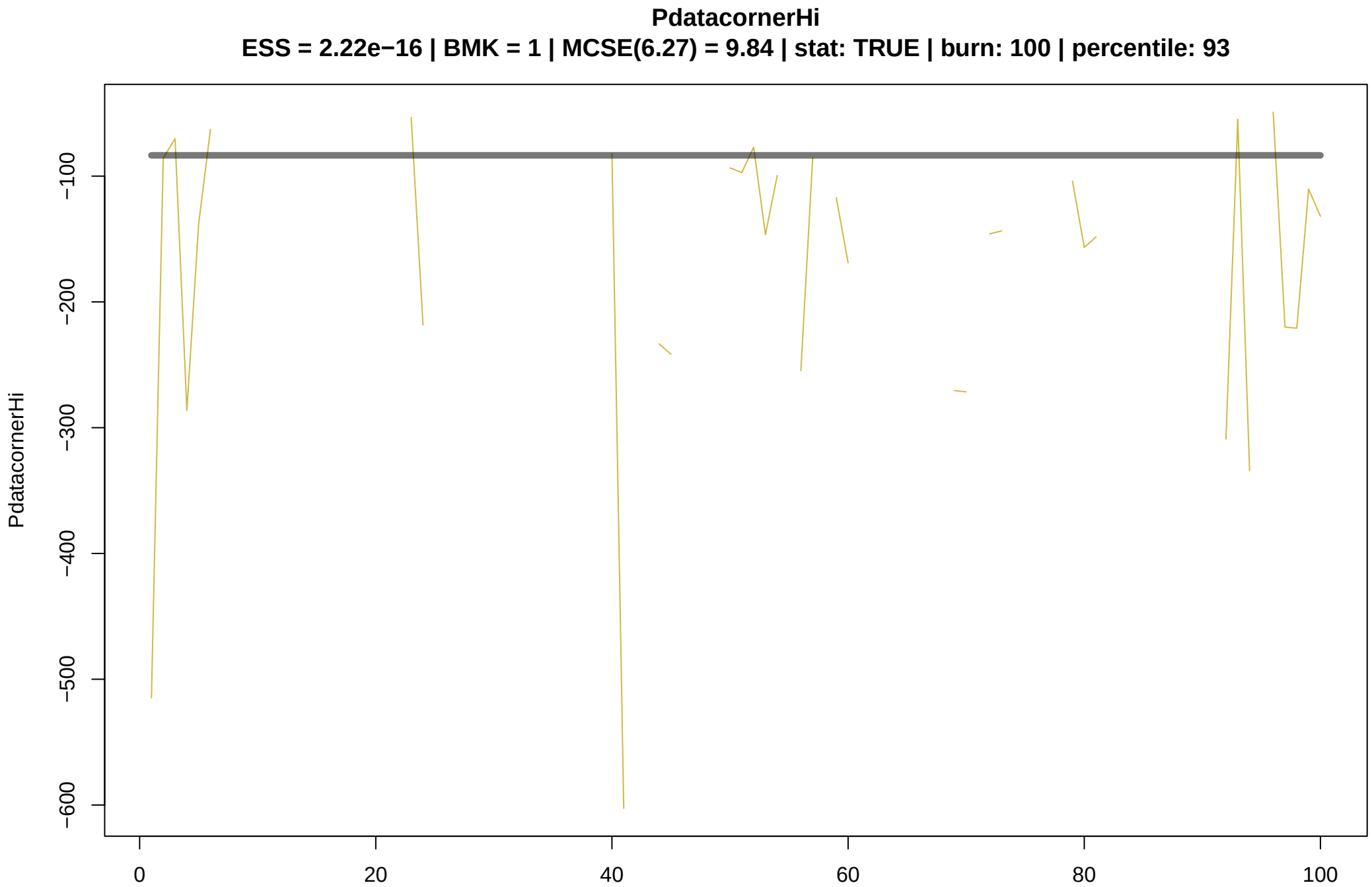

docked_NumRotatableBonds
100
80
60
40
20
0
−300
−100
0
100
300
log_RMSD

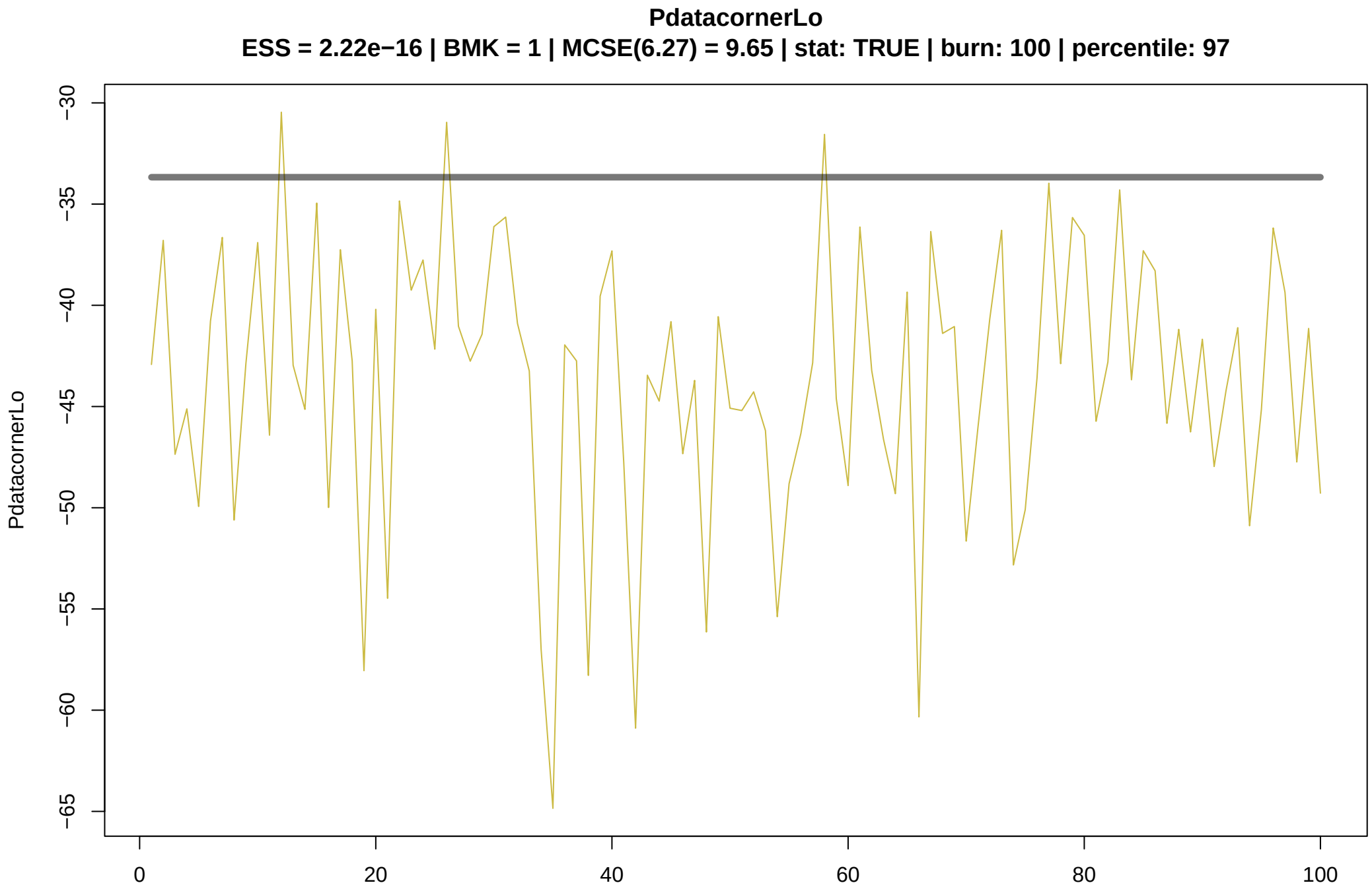

mcs_NOCount
120
100
80
60
40
20
0
−300
−100
0
100
300
log_RMSD

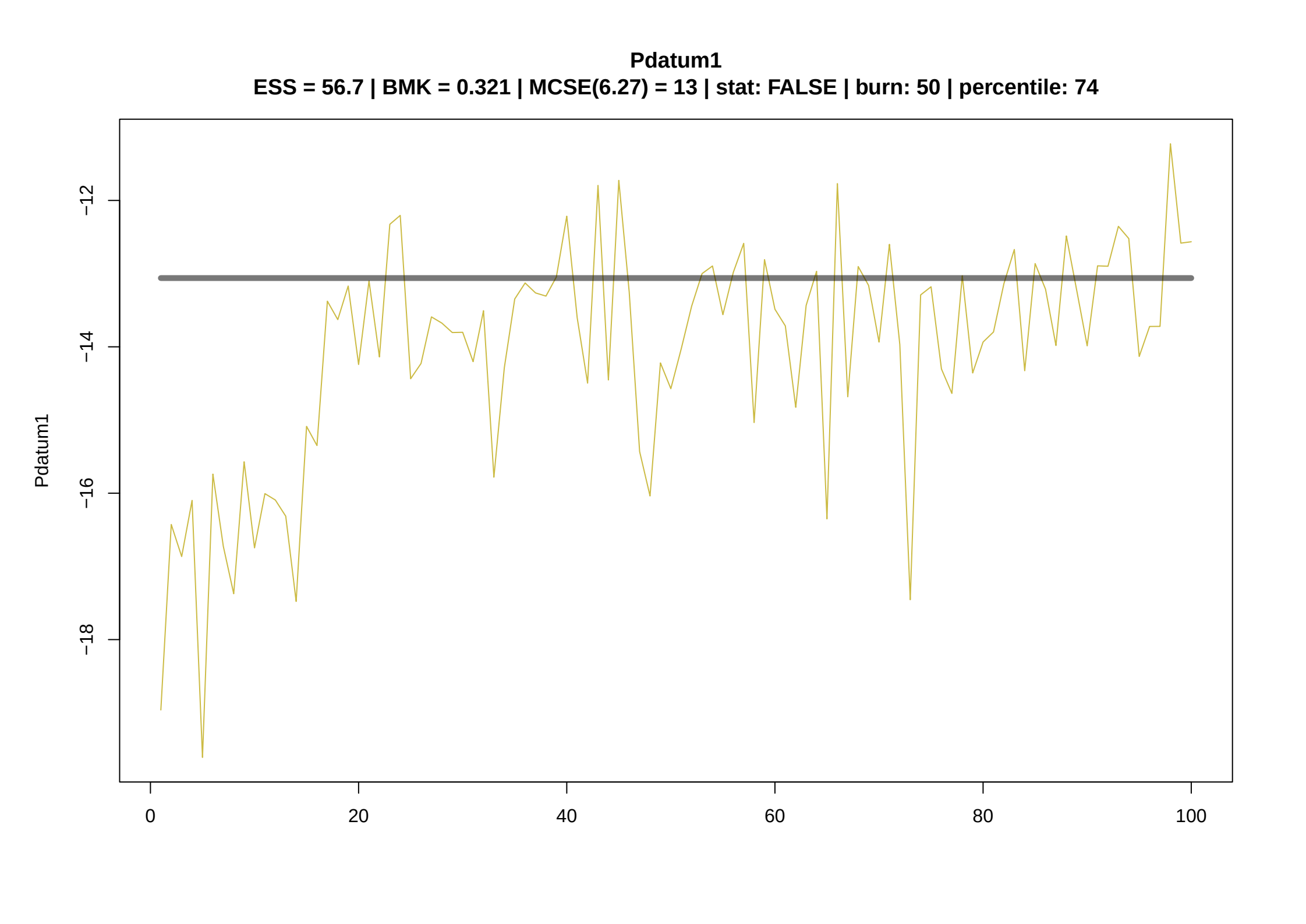

LL
LL
−230
−240
−250
−260
−270
−280
0
20
40
60
80
100

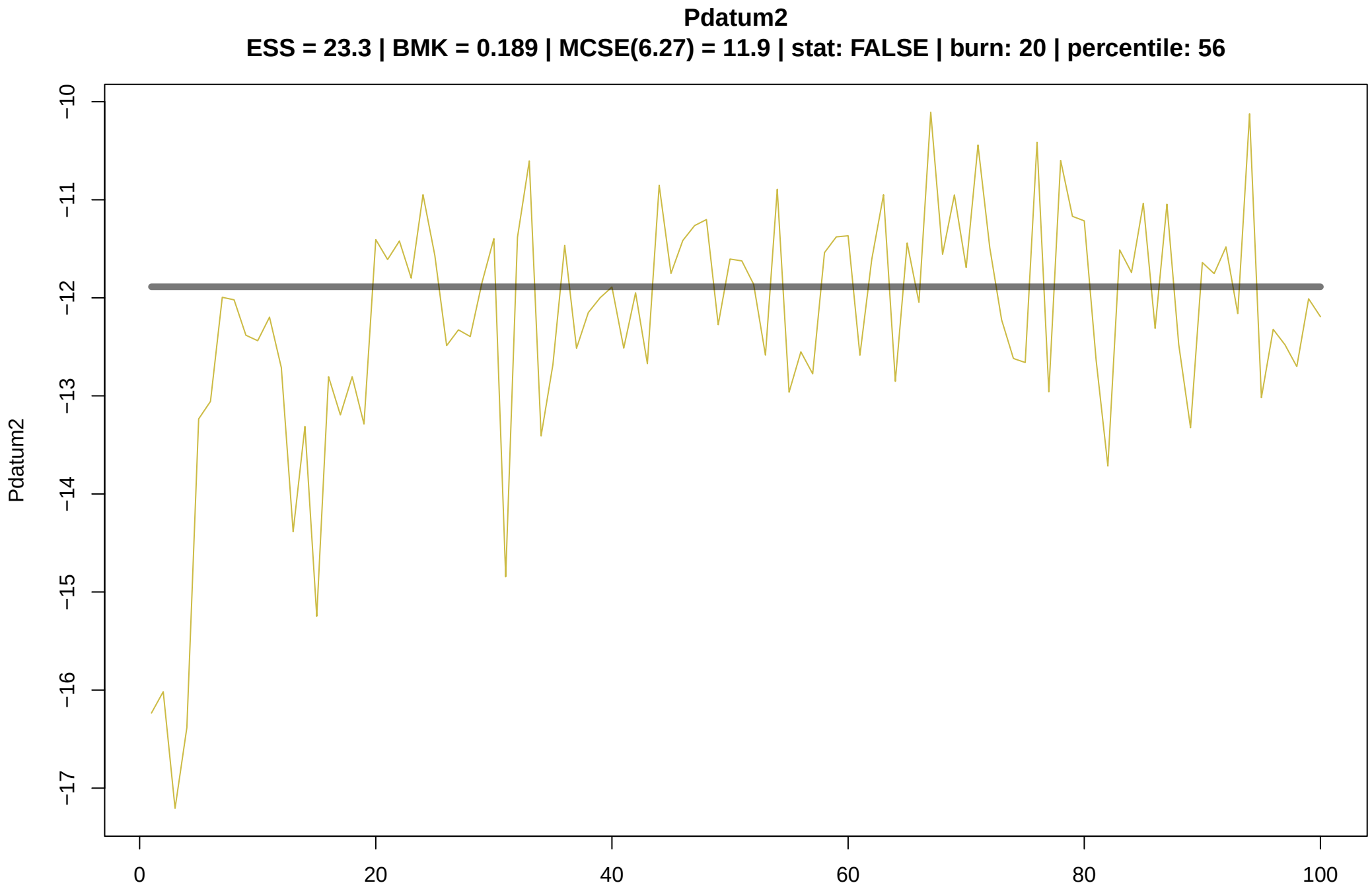

alpha
alpha
1
2
3
4
0
20
40
60
80
100

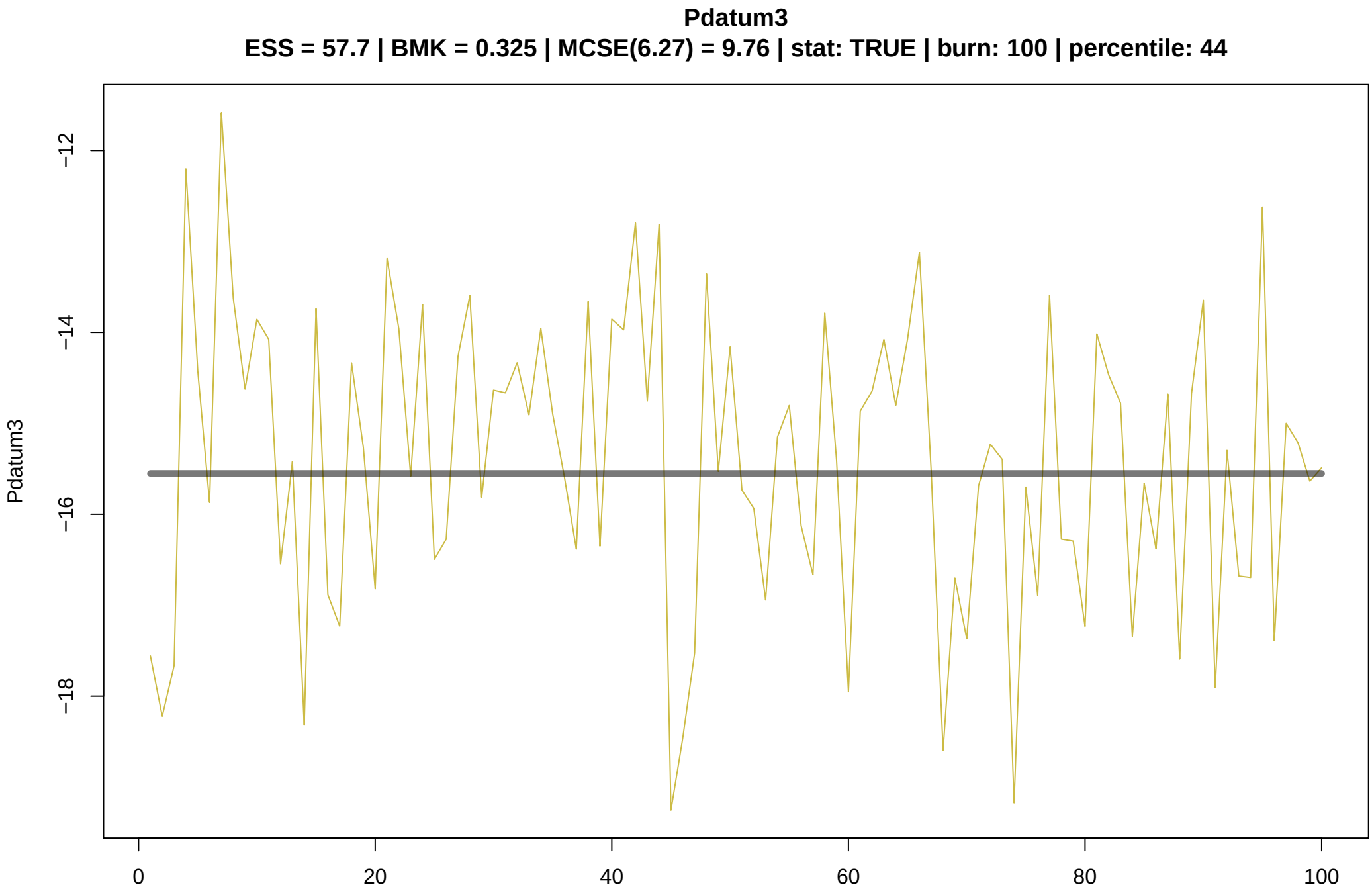

Pdatamean
ESS = 70.8 | BMK = 1 | MCSE(6.27) = 14.3 | stat: TRUE | burn: 100 | percentile: 70
Pdatamean
−20
−30
−40
−50
−60
0
20
40
60
80
100

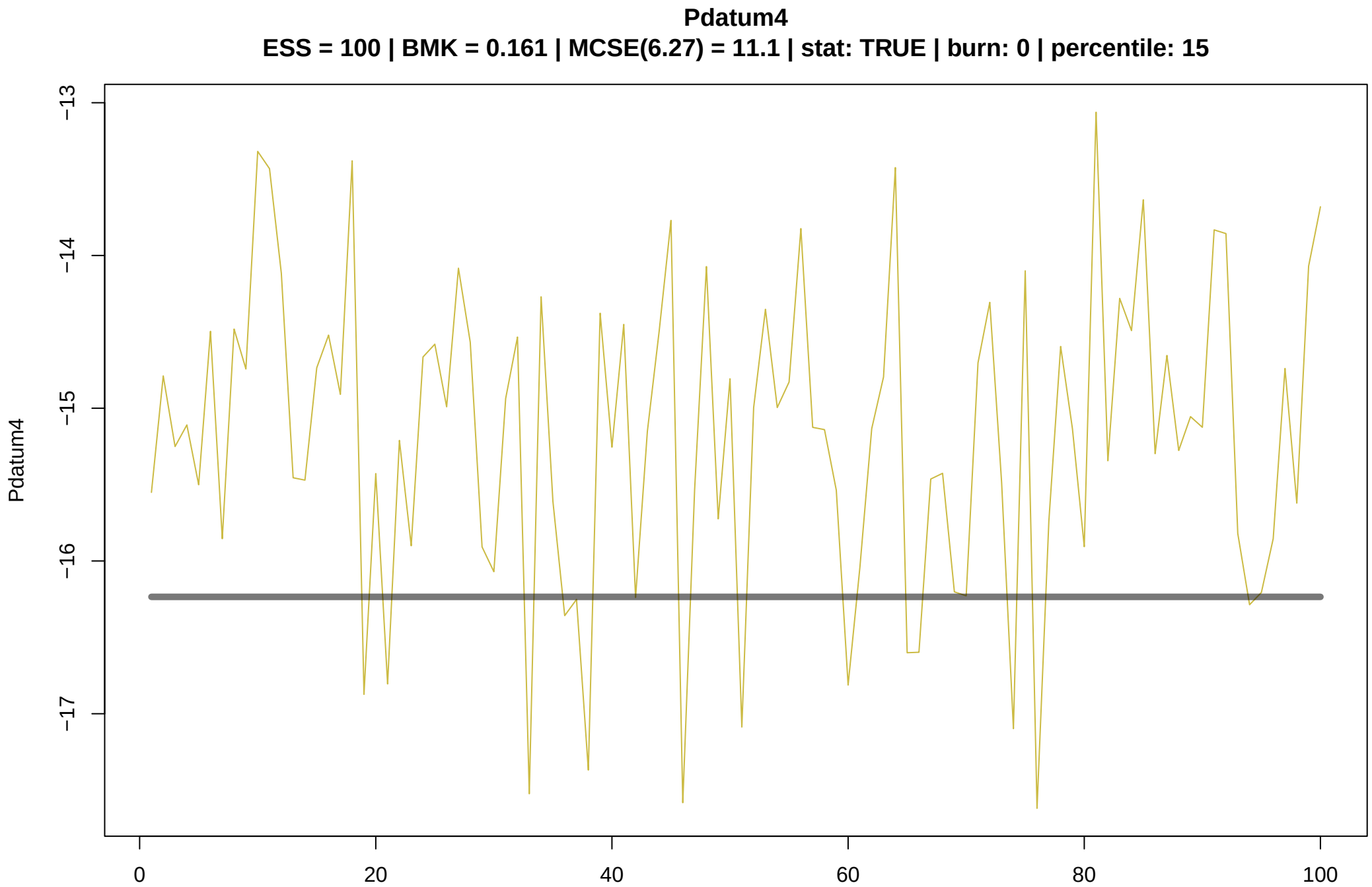

PdatacornerHi
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 9.84 | stat: TRUE | burn: 100 | percentile: 93
PdatacornerHi
−100
−200
−300
−400
−500
−600
0
20
40
60
80
100

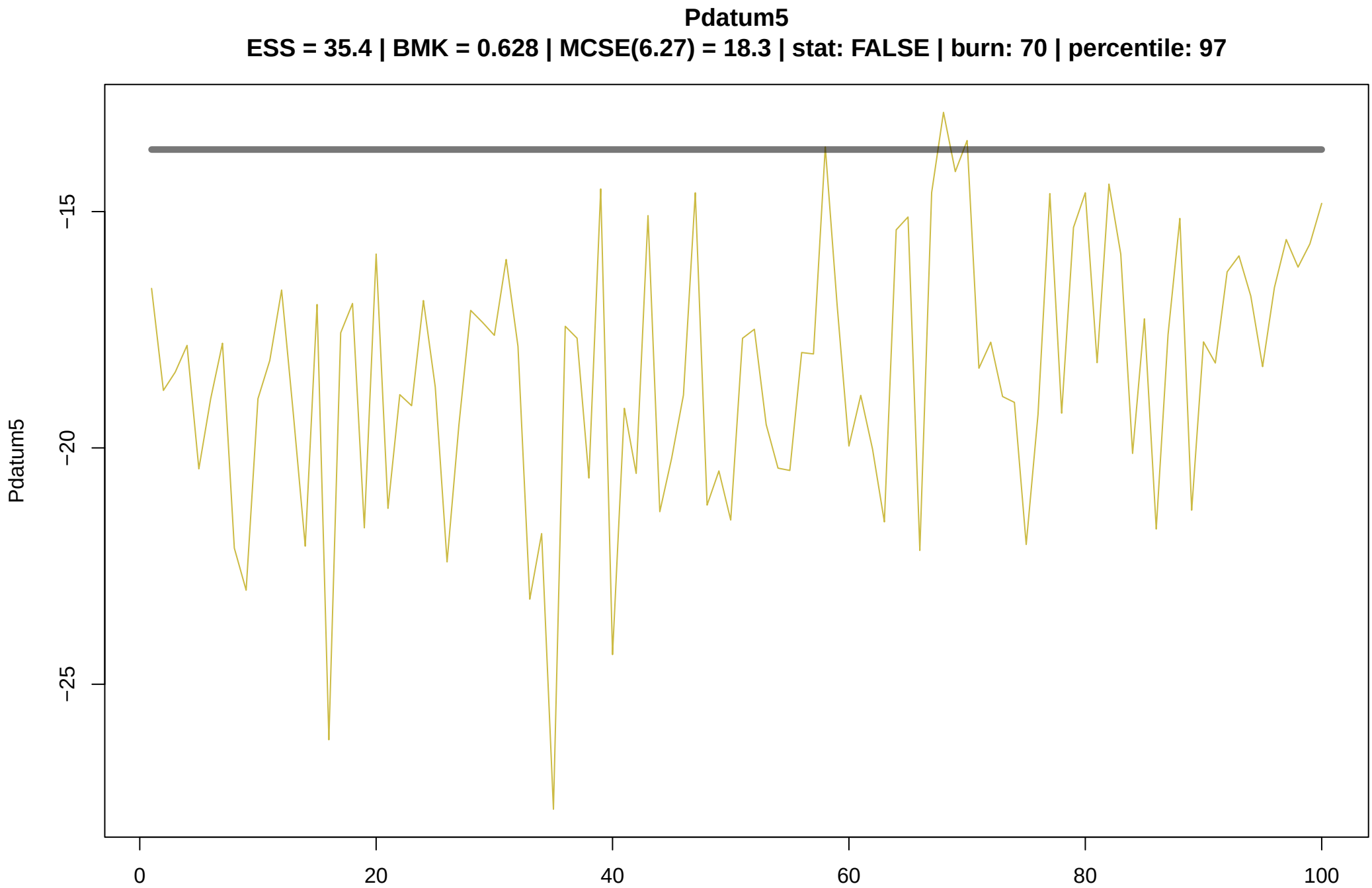

PdatacornerLo
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 9.65 | stat: TRUE | burn: 100 | percentile: 97
PdatacornerLo
−30
−35
−40
−45
−50
−55
−60
−65
0
20
40
60
80
100

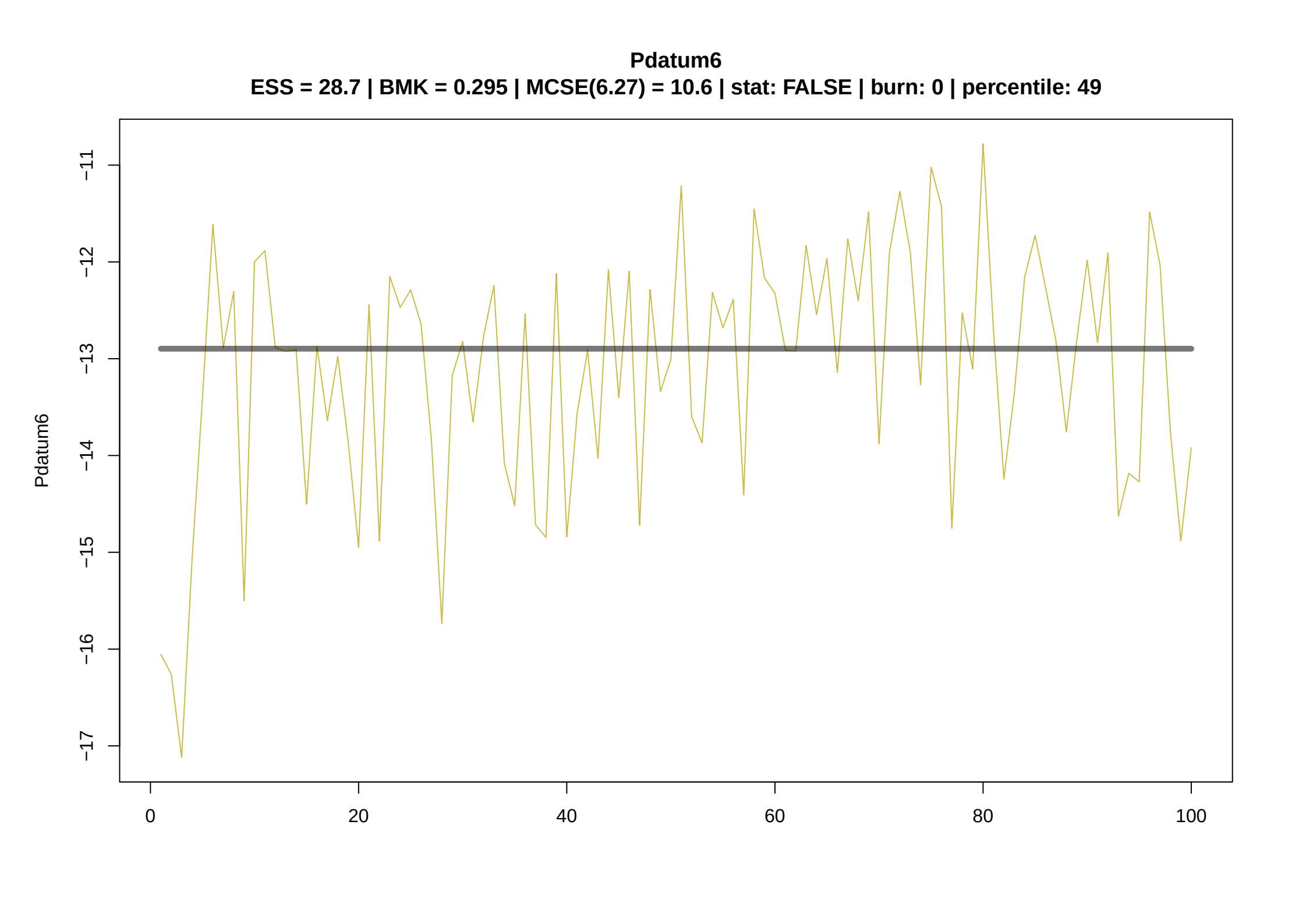

Pdatum1
ESS = 56.7 | BMK = 0.321 | MCSE(6.27) = 13 | stat: FALSE | burn: 50 | percentile: 74
Pdatum1
−12
−14
−16
−18
0
20
40
60
80
100

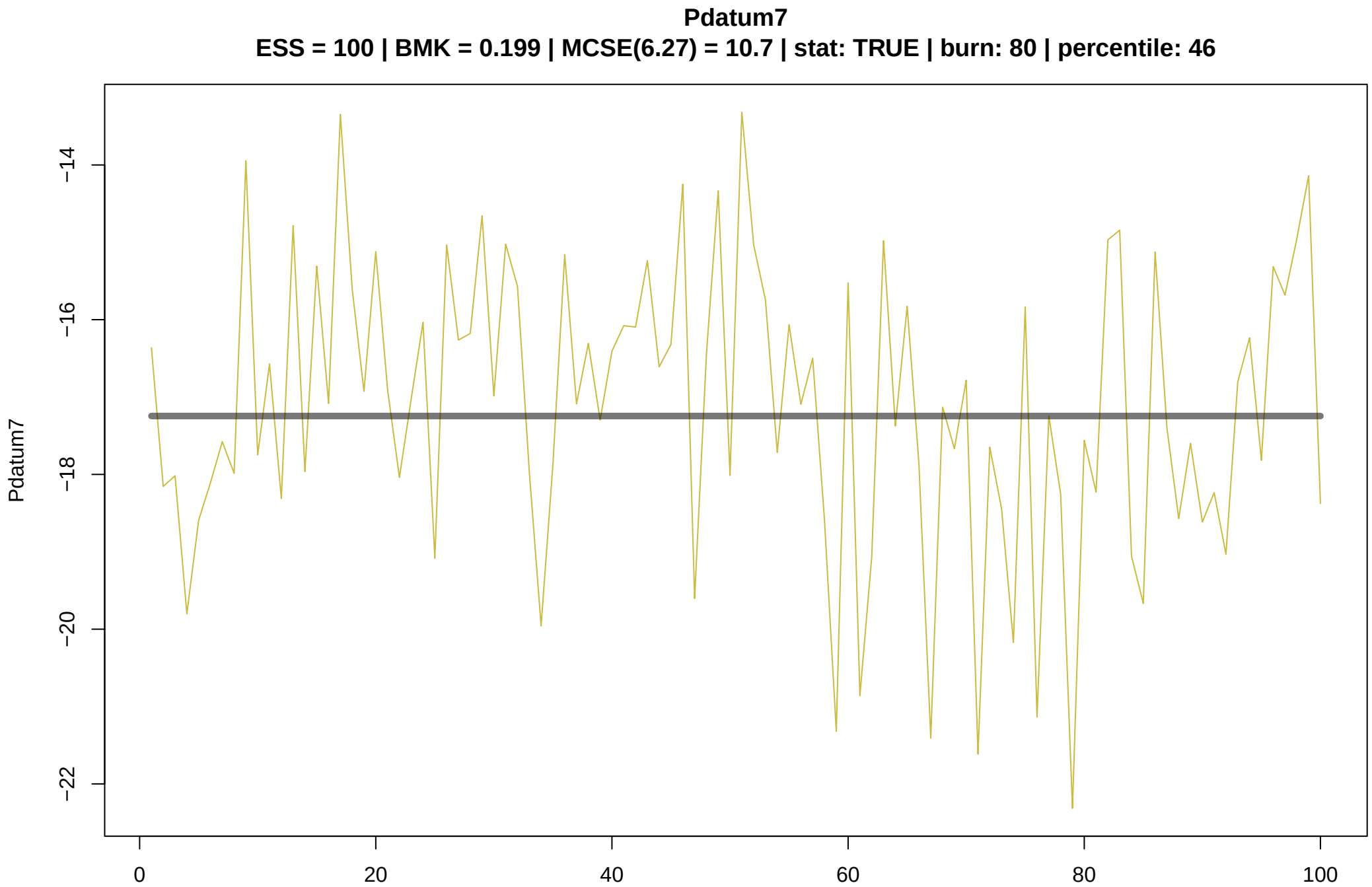

Pdatum2
ESS = 23.3 | BMK = 0.189 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 20 | percentile: 56
Pdatum2
−10
−11
−12
−13
−14
−15
−16
−17
0
20
40
60
80
100

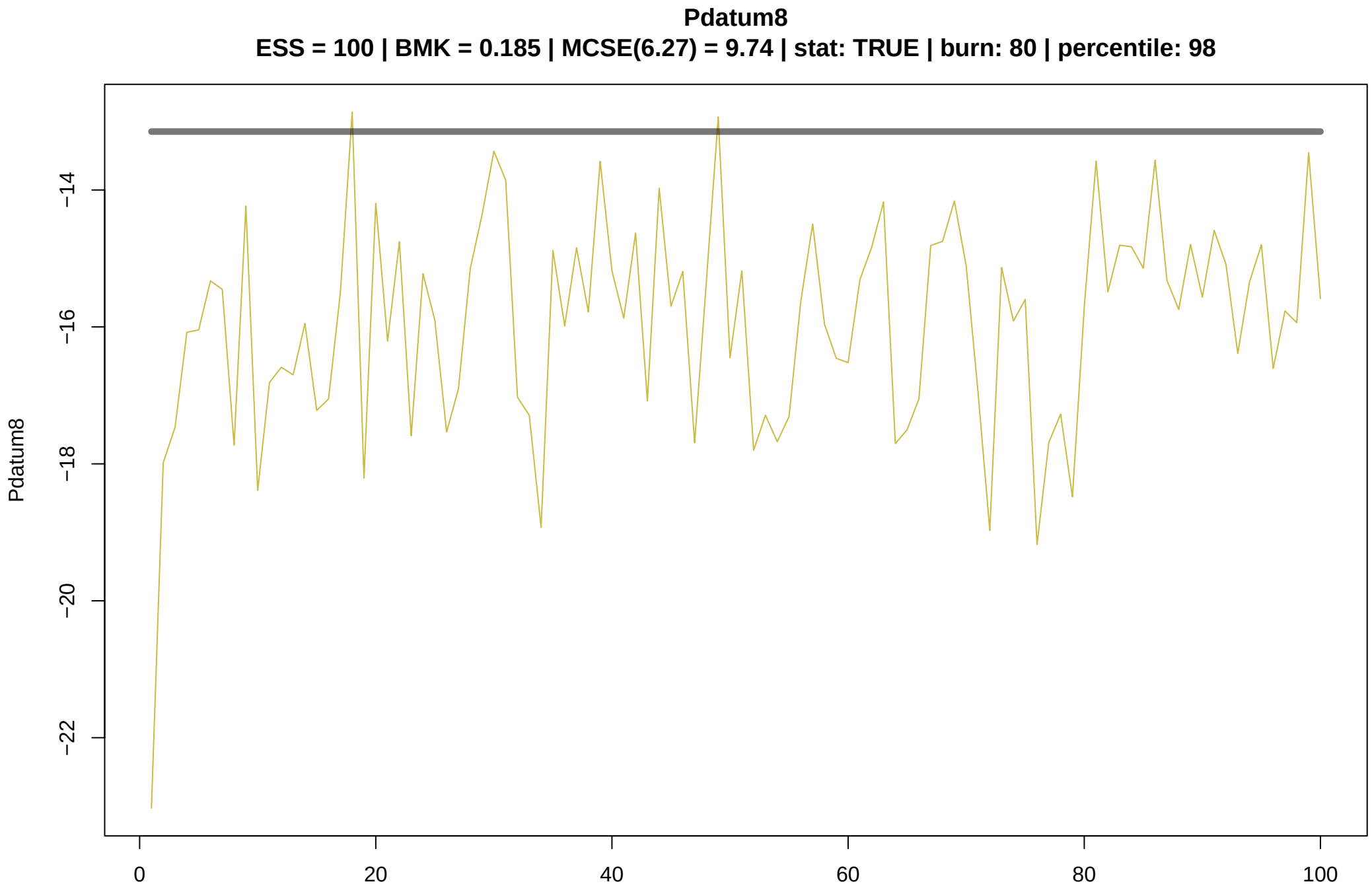

Pdatum3
ESS = 57.7 | BMK = 0.325 | MCSE(6.27) = 9.76 | stat: TRUE | burn: 100 | percentile: 44
Pdatum3
−12
−14
−16
−18
0
20
40
60
80
100

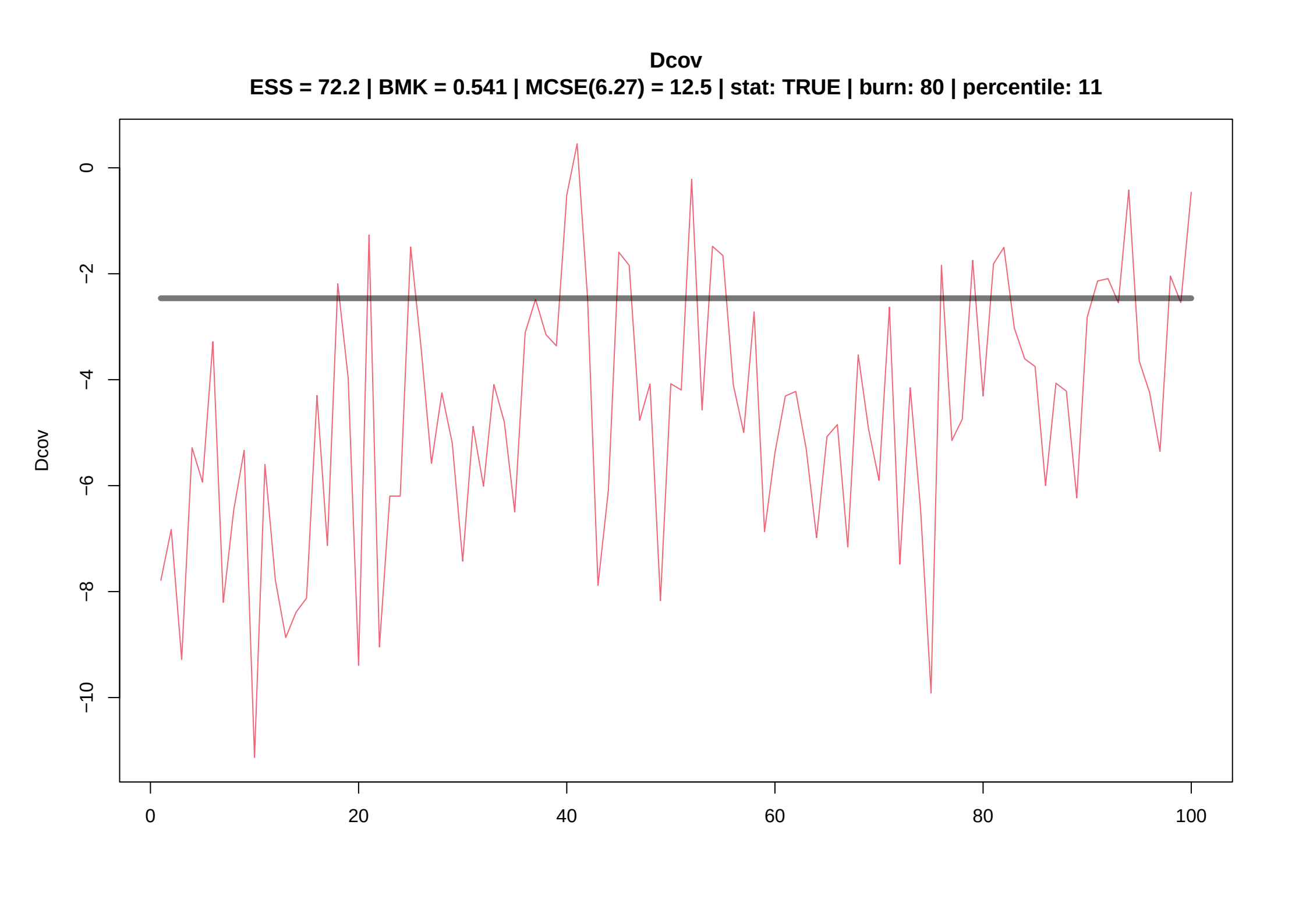

Pdatum4
ESS = 100 | BMK = 0.161 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0 | percentile: 15
Pdatum4
−13
−14
−15
−16
−17
0
20
40
60
80
100

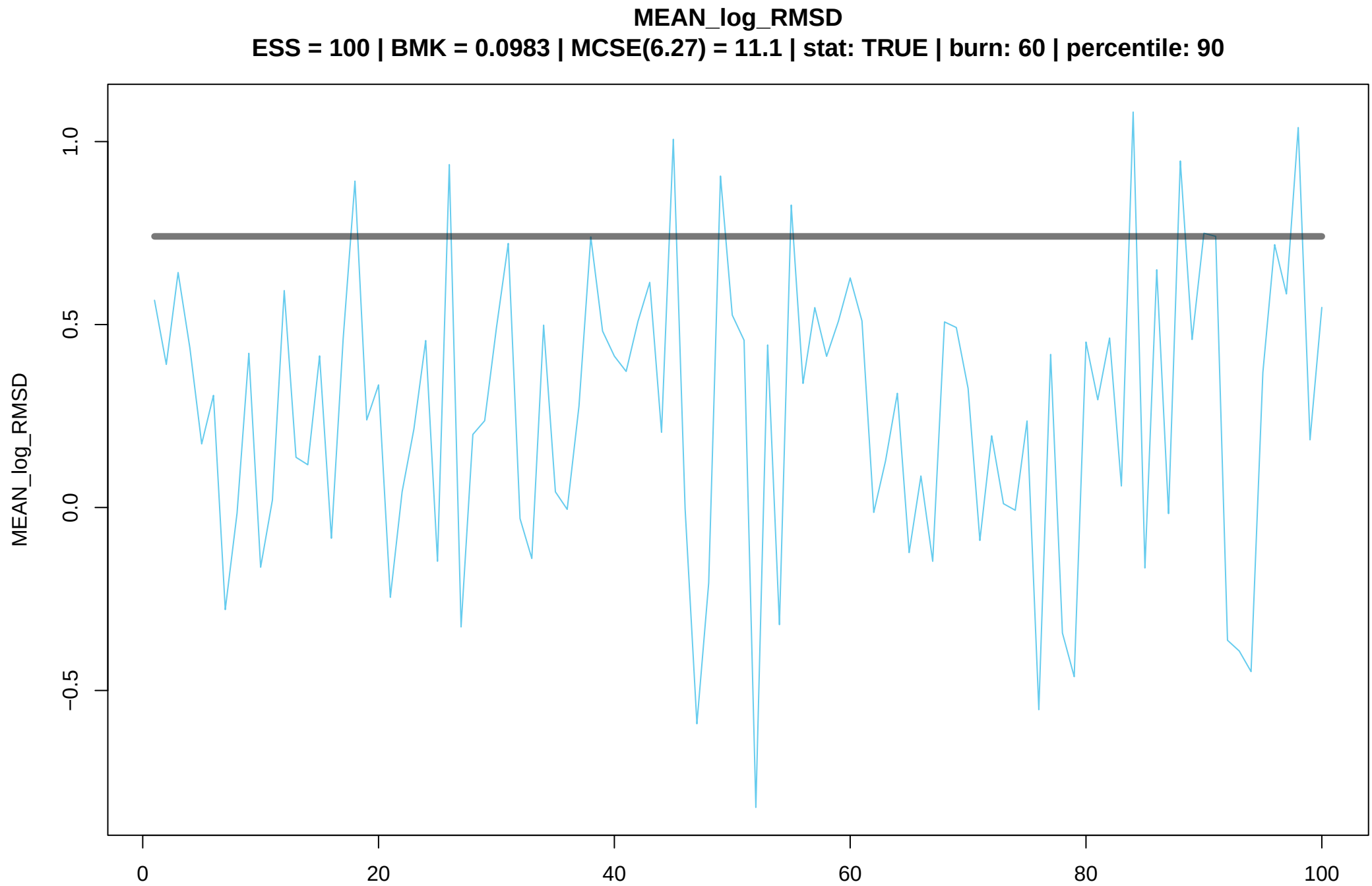

Pdatum5
ESS = 35.4 | BMK = 0.628 | MCSE(6.27) = 18.3 | stat: FALSE | burn: 70 | percentile: 97
Pdatum5
−15
−20
−25
0
20
40
60
80
100

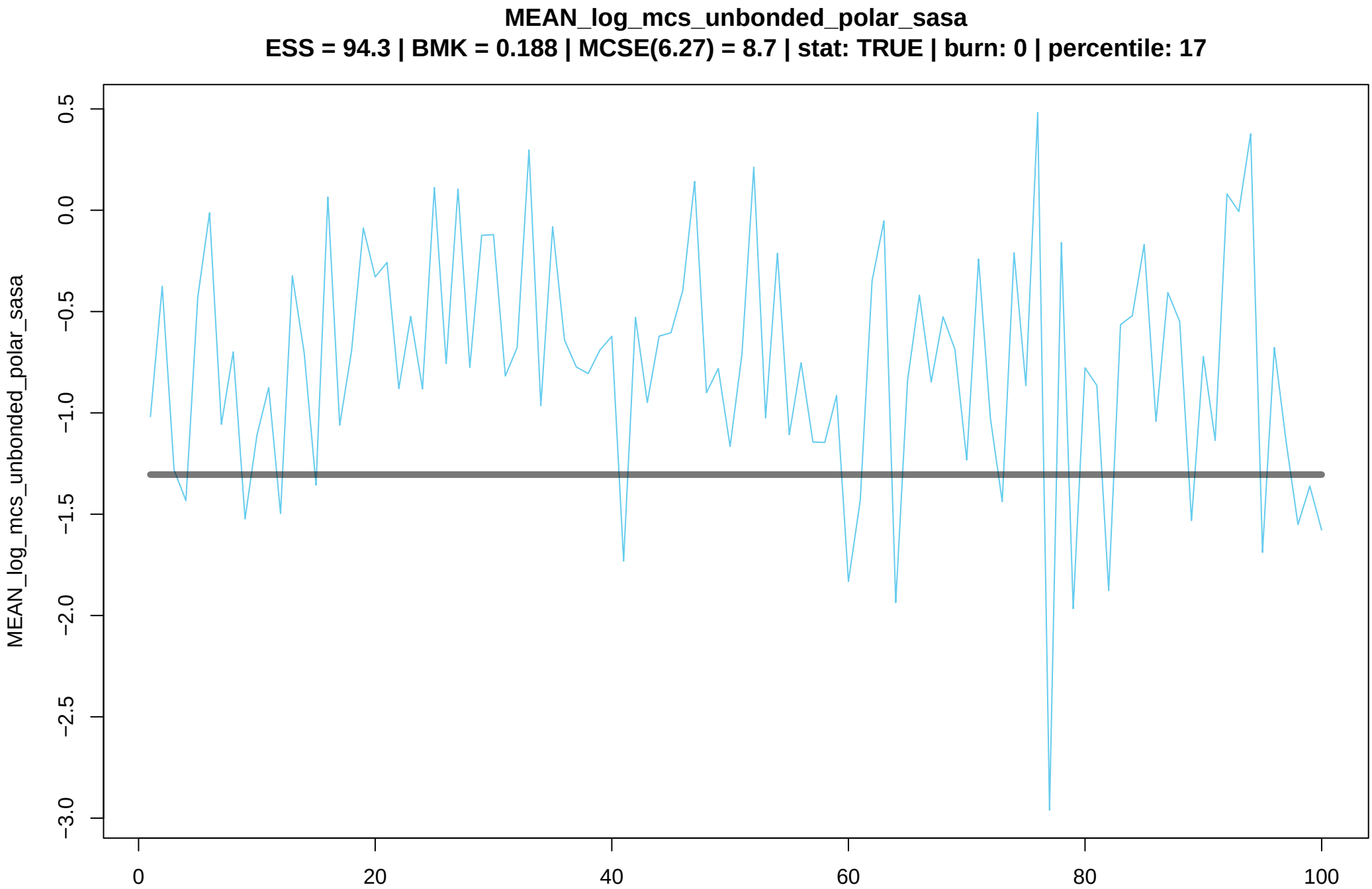

Pdatum6
ESS = 28.7 | BMK = 0.295 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 0 | percentile: 49
Pdatum6
−11
−12
−13
−14
−15
−16
−17
0
20
40
60
80
100

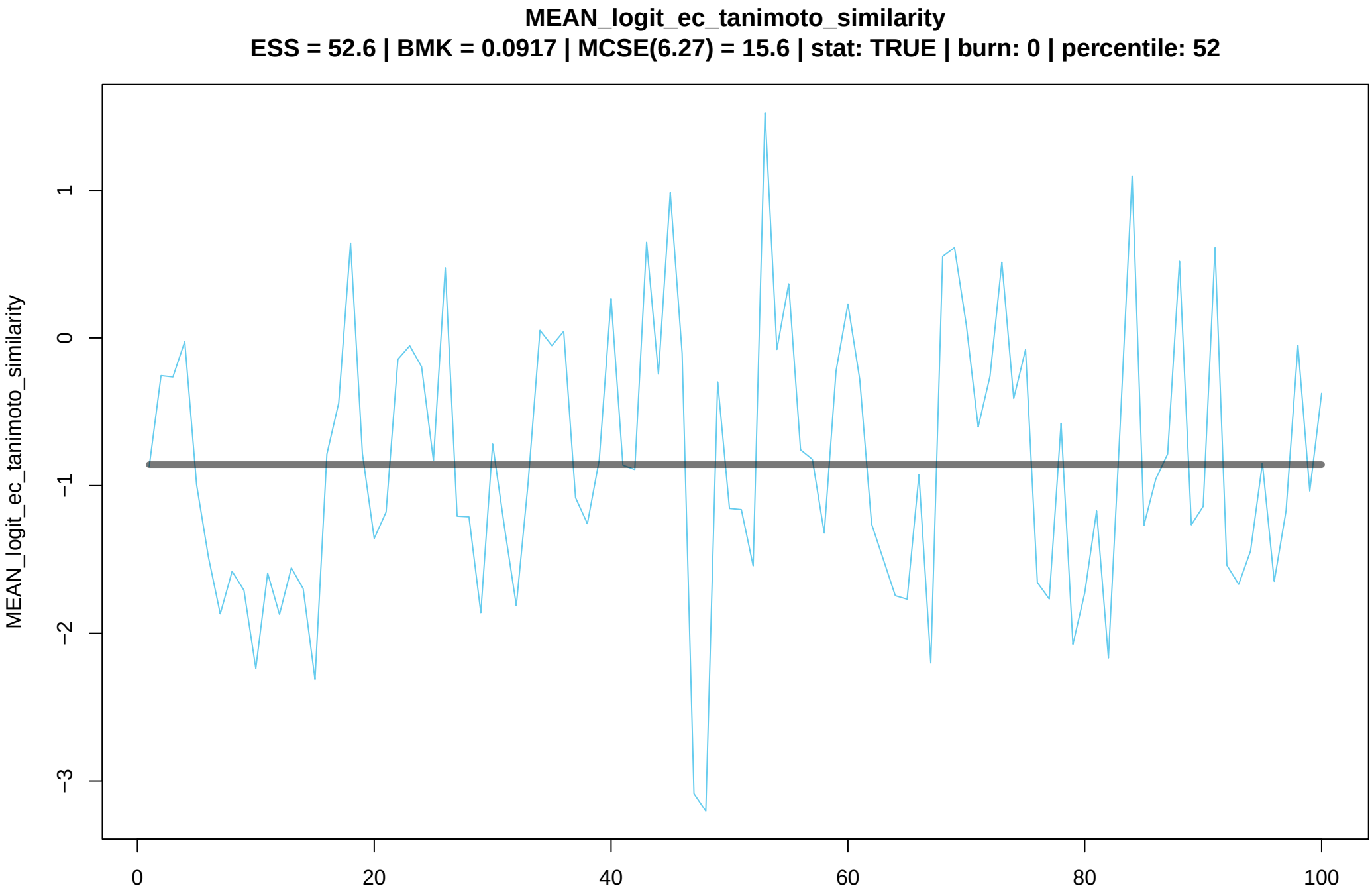

Pdatum7
ESS = 100 | BMK = 0.199 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 80 | percentile: 46
Pdatum7
−14
−16
−18
−20
−22
0
20
40
60
80
100

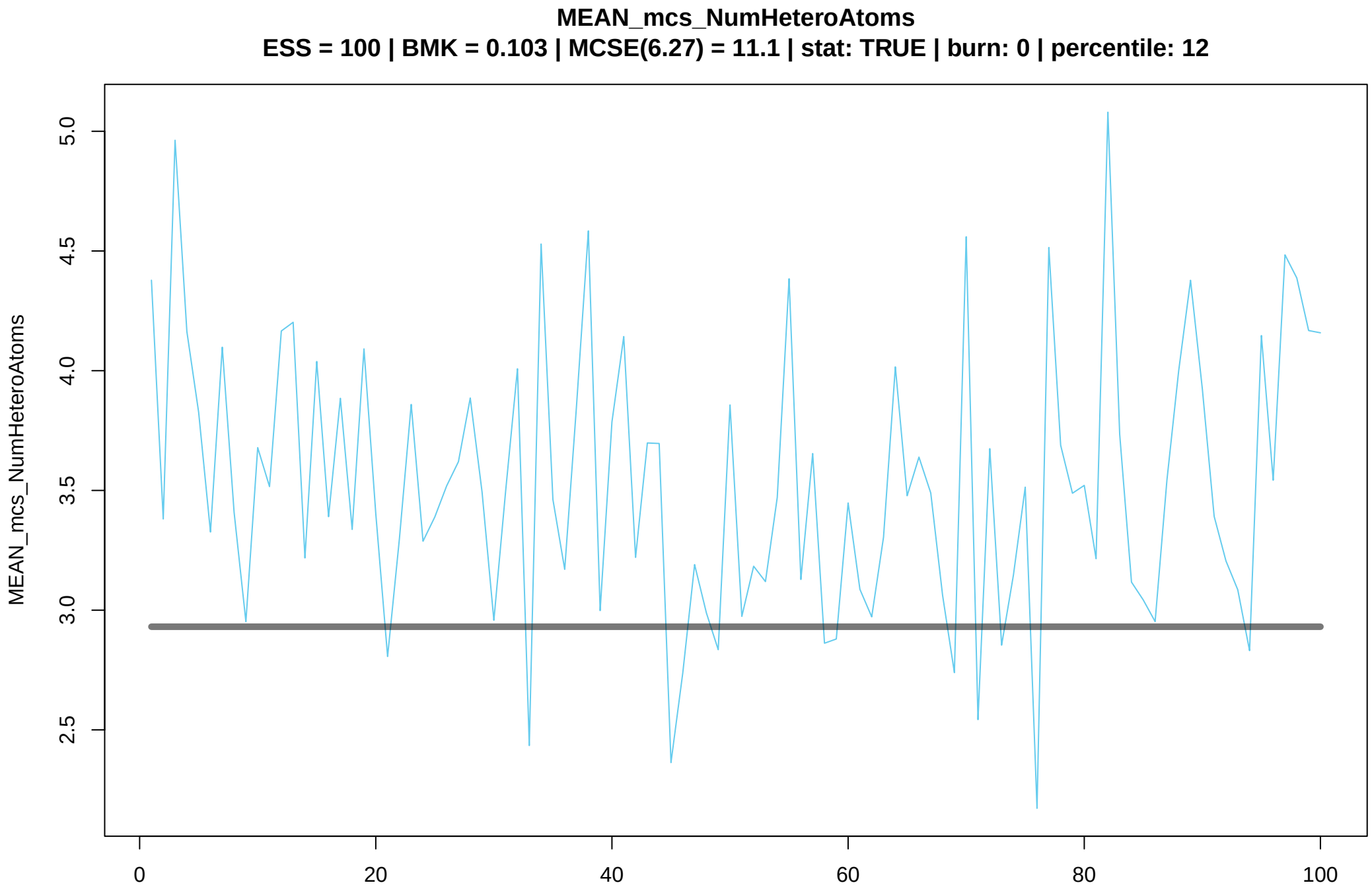

Pdatum8
ESS = 100 | BMK = 0.185 | MCSE(6.27) = 9.74 | stat: TRUE | burn: 80 | percentile: 98
Pdatum8
−14
−16
−18
−20
−22
0
20
40
60
80
100

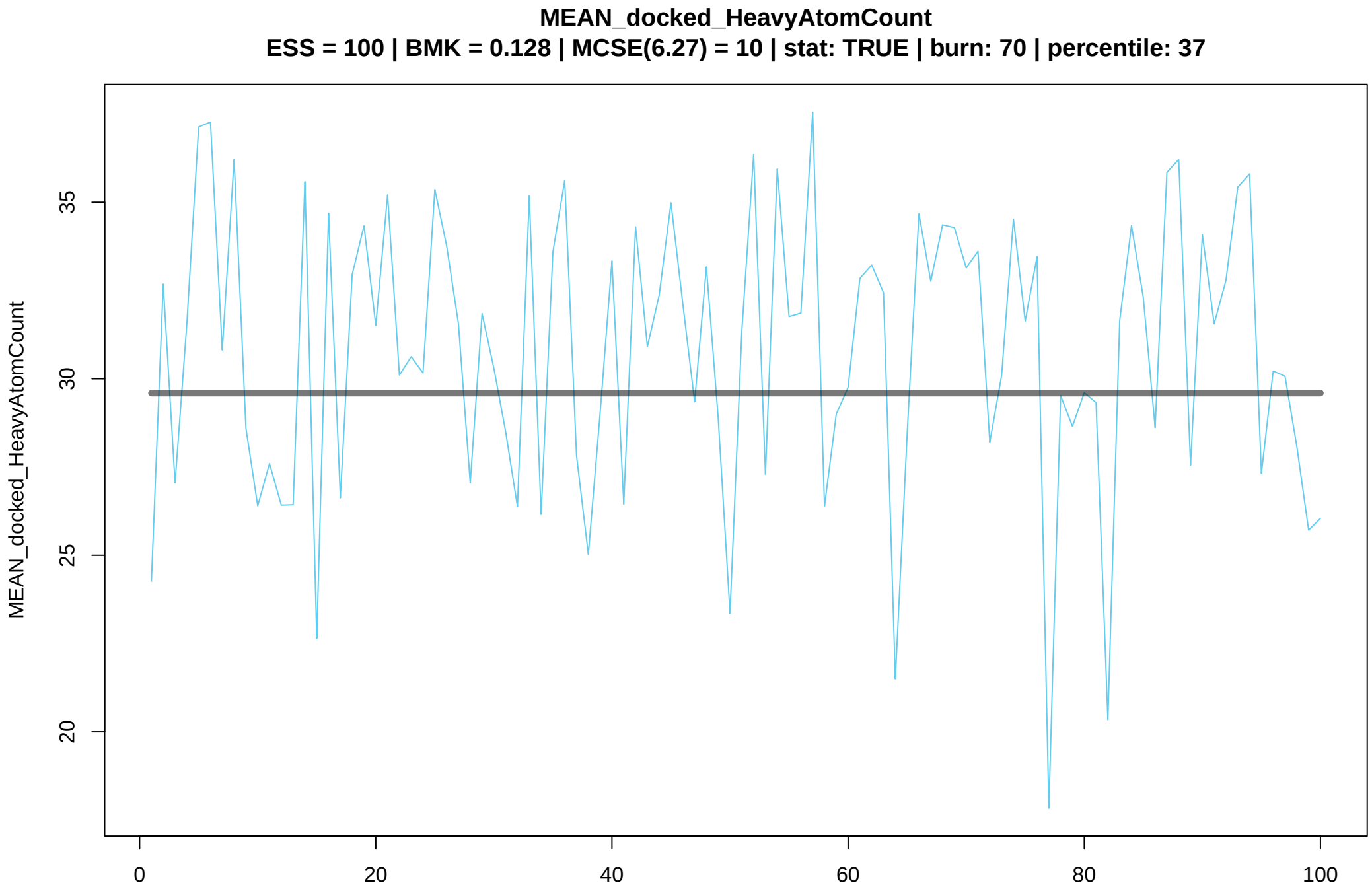

Dcov
ESS = 72.2 | BMK = 0.541 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 80 | percentile: 11
Dcov
0
−2
−4
−6
−8
−10
0
20
40
60
80
100

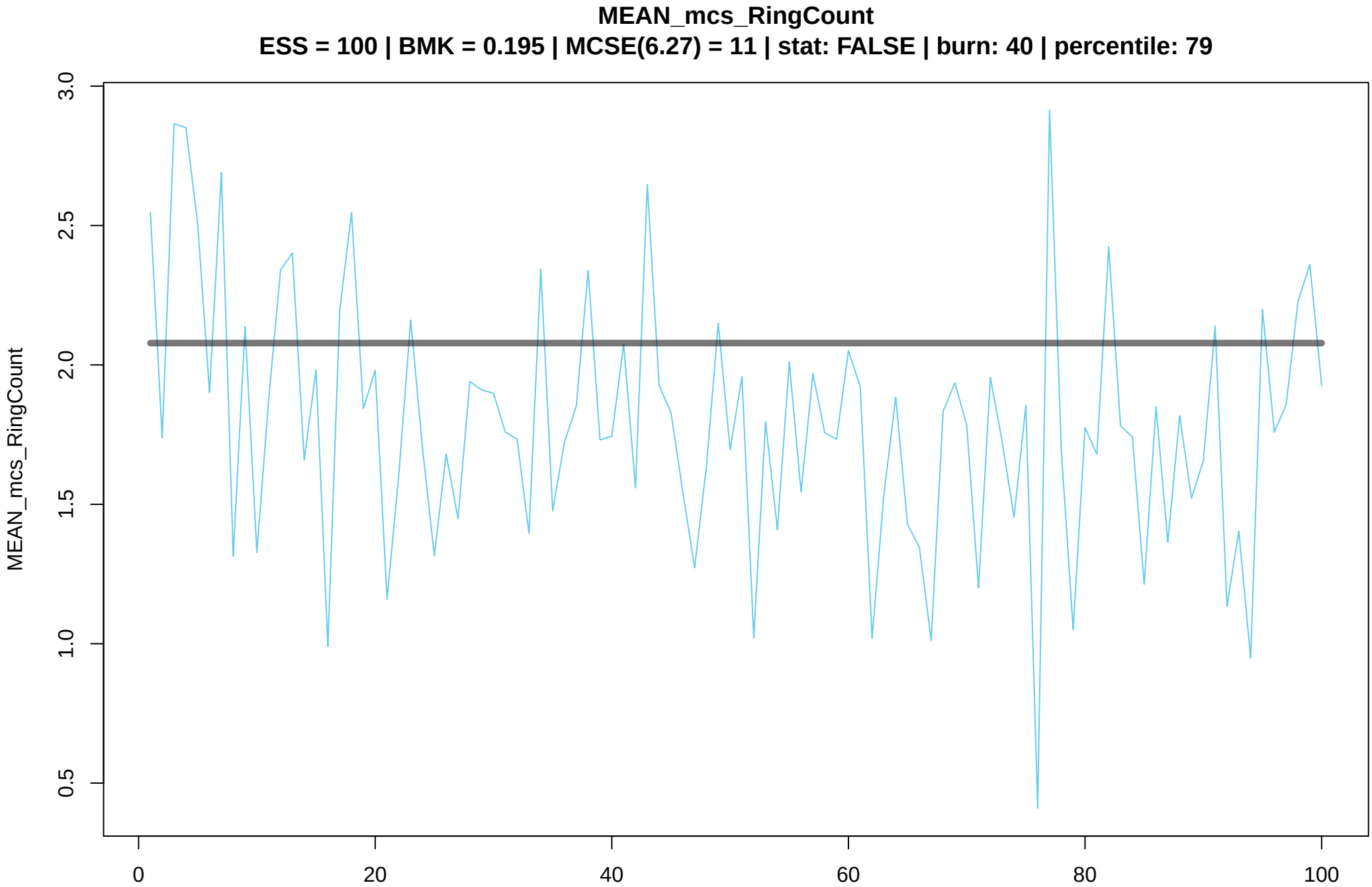

MEAN_log_RMSD
ESS = 100 | BMK = 0.0983 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 60 | percentile: 90
MEAN_log_RMSD
1.0
0.5
0.0
−0.5
0
20
40
60
80
100

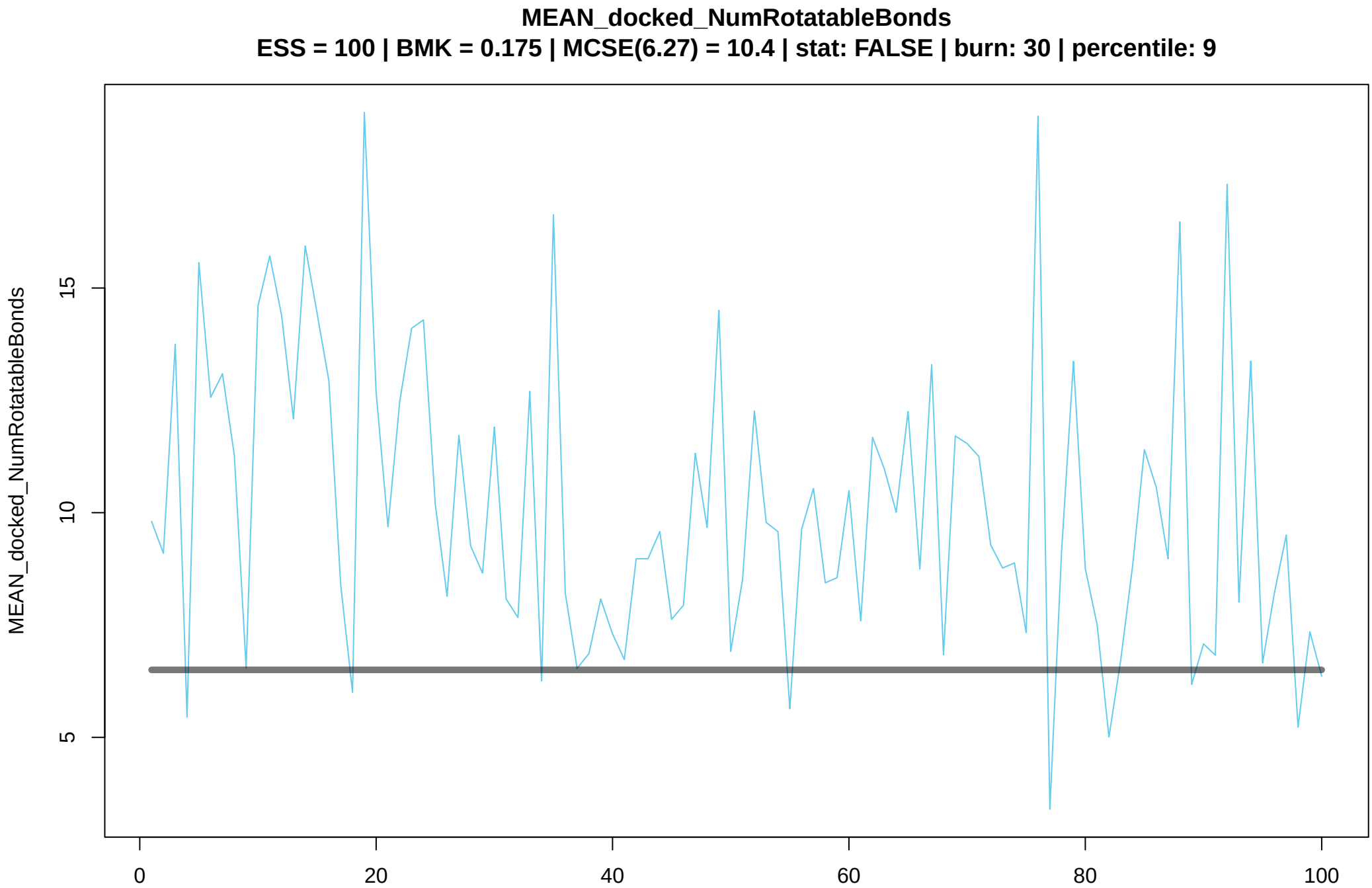

MEAN_log_mcs_unbonded_polar_sasa
ESS = 94.3 | BMK = 0.188 | MCSE(6.27) = 8.7 | stat: TRUE | burn: 0 | percentile: 17
MEAN_log_mcs_unbonded_polar_sasa
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
0
20
40
60
80
100

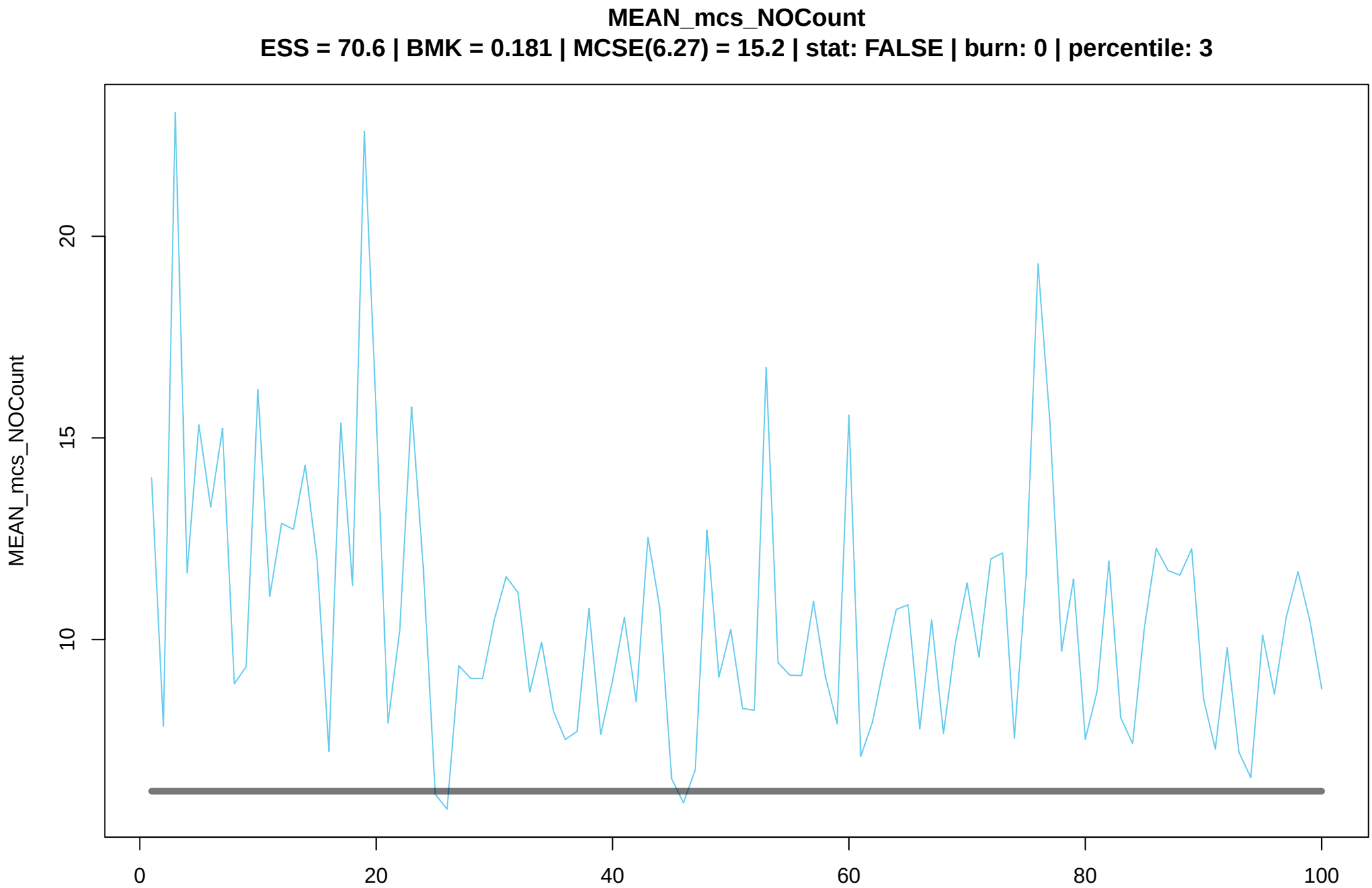

MEAN_logit_ec_tanimoto_similarity
ESS = 52.6 | BMK = 0.0917 | MCSE(6.27) = 15.6 | stat: TRUE | burn: 0 | percentile: 52
MEAN_logit_ec_tanimoto_similarity
1
0
−1
−2
−3
0
20
40
60
80
100

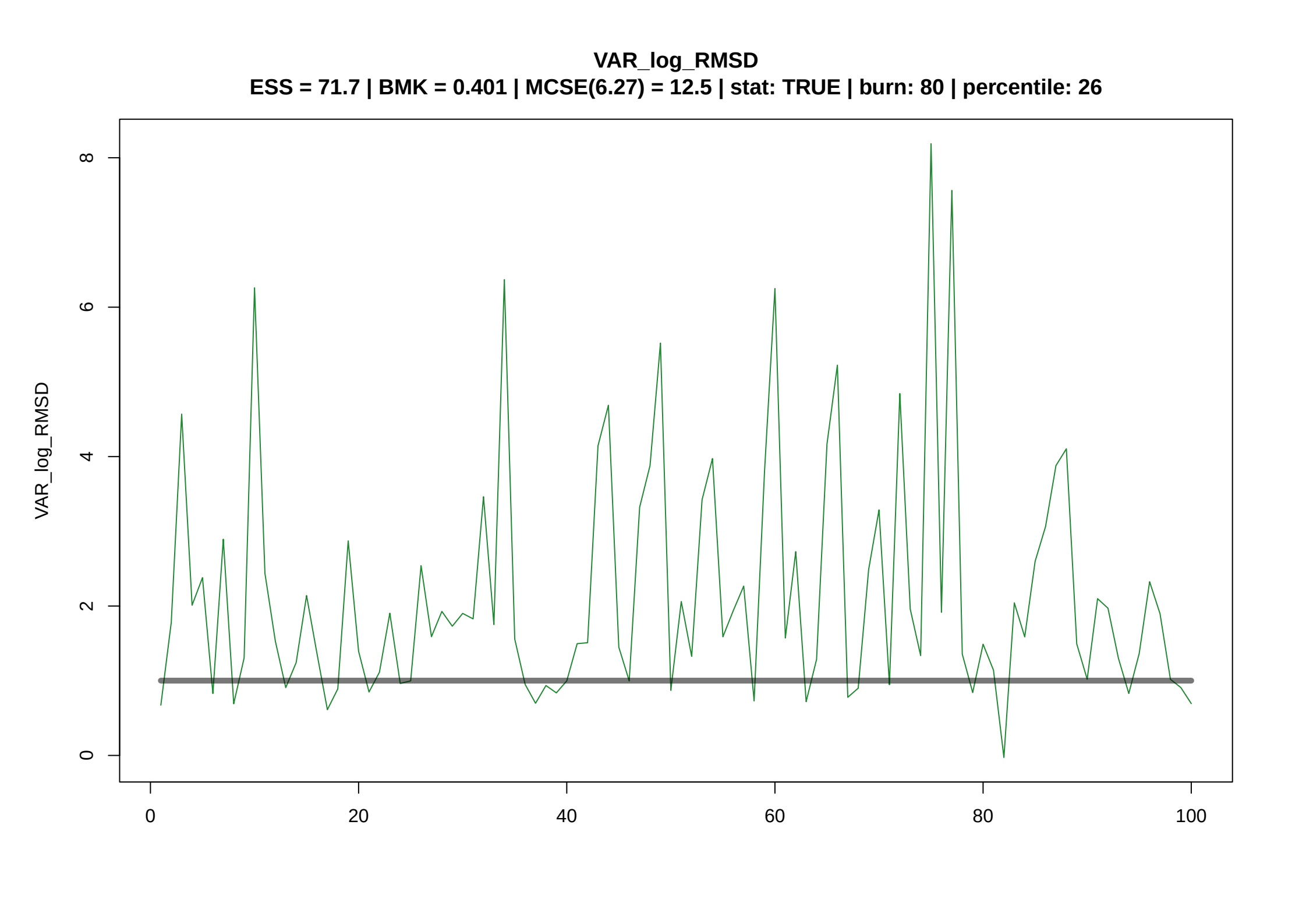

MEAN_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.103 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0 | percentile: 12
MEAN_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
0
20
40
60
80
100

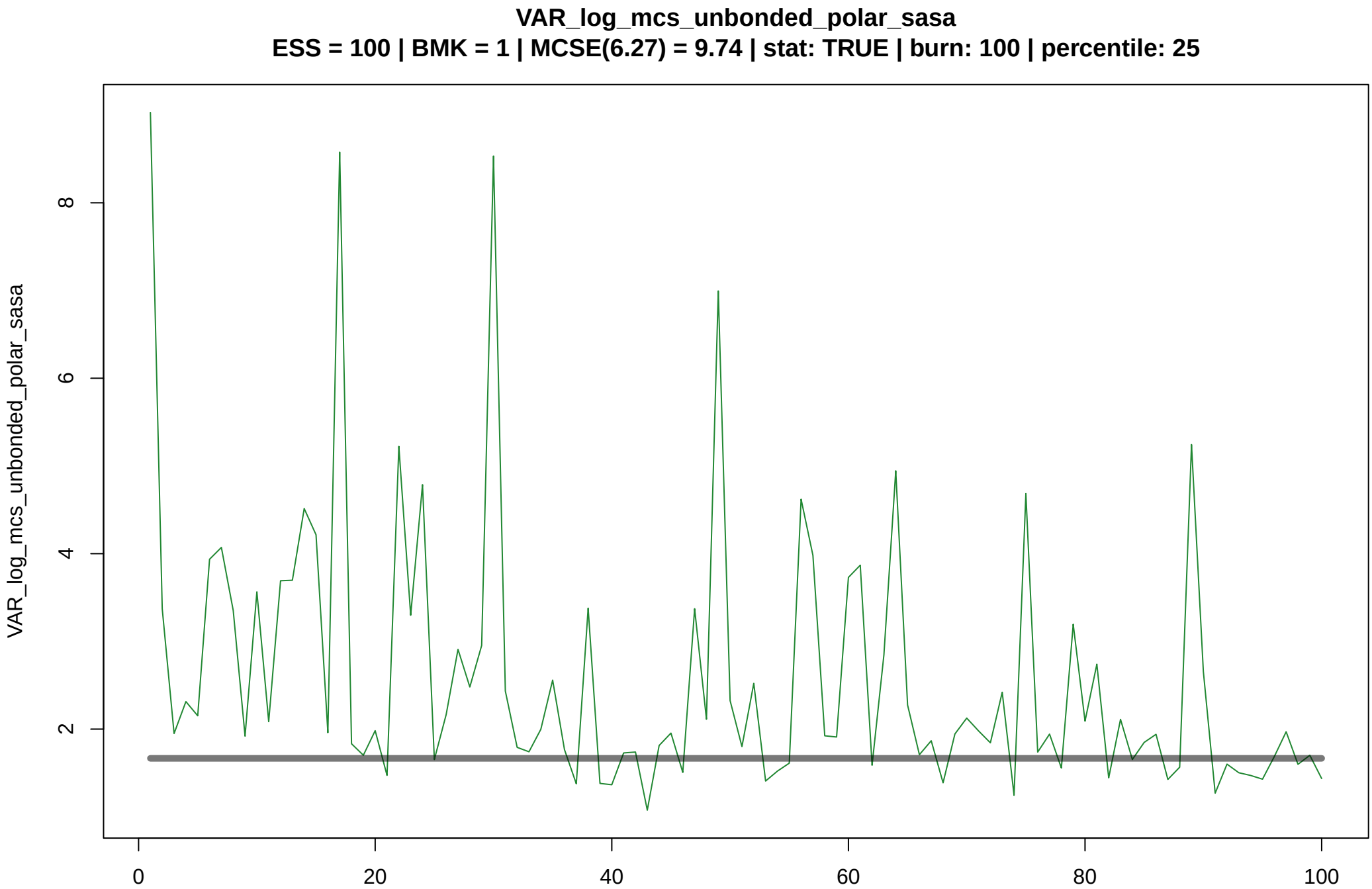

MEAN_docked_HeavyAtomCount
ESS = 100 | BMK = 0.128 | MCSE(6.27) = 10 | stat: TRUE | burn: 70 | percentile: 37
MEAN_docked_HeavyAtomCount
20
25
30
35
0
20
40
60
80
100

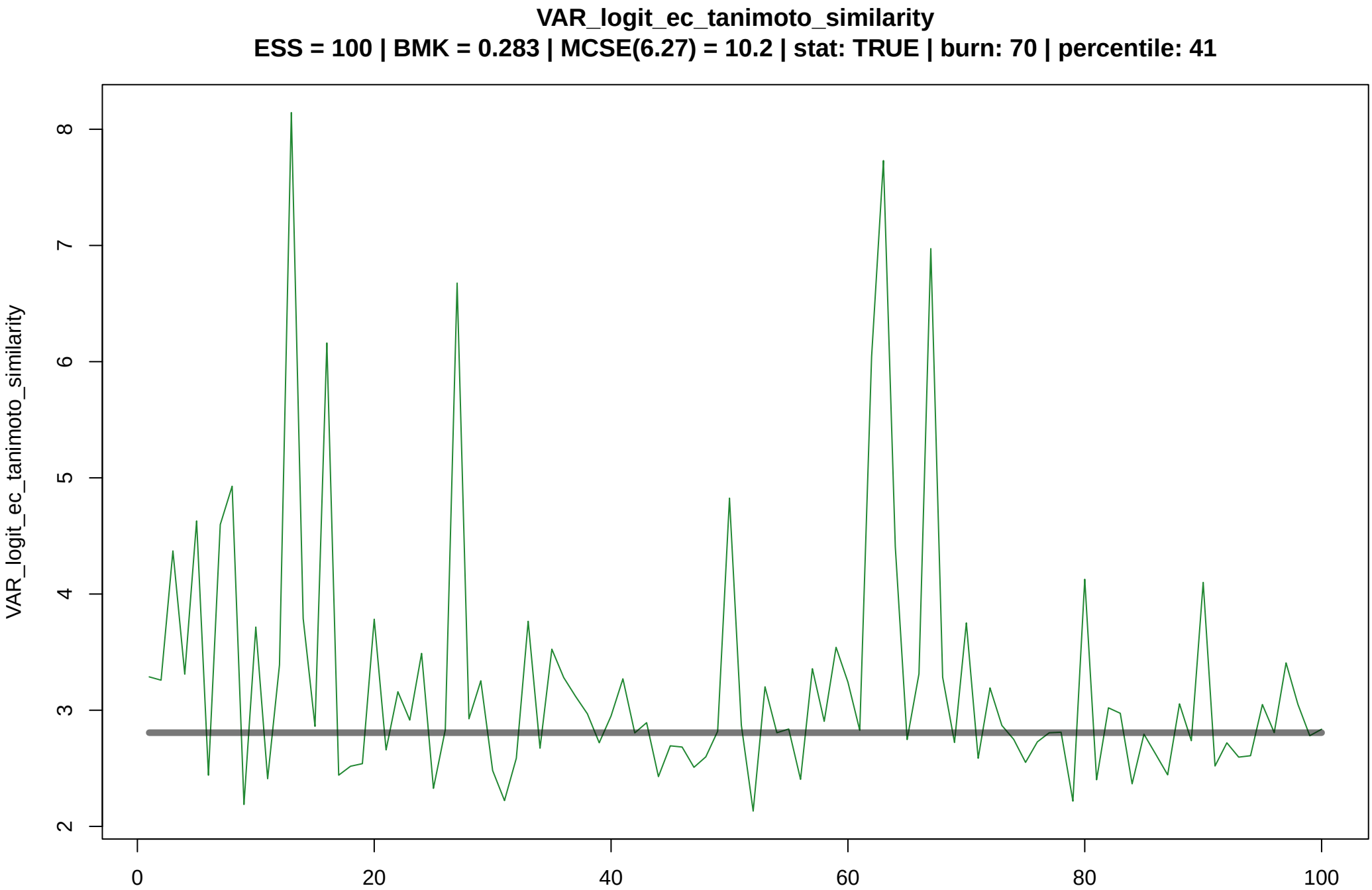

MEAN_mcs_RingCount
ESS = 100 | BMK = 0.195 | MCSE(6.27) = 11 | stat: FALSE | burn: 40 | percentile: 79
MEAN_mcs_RingCount
3.0
2.5
2.0
1.5
1.0
0.5
0
20
40
60
80
100

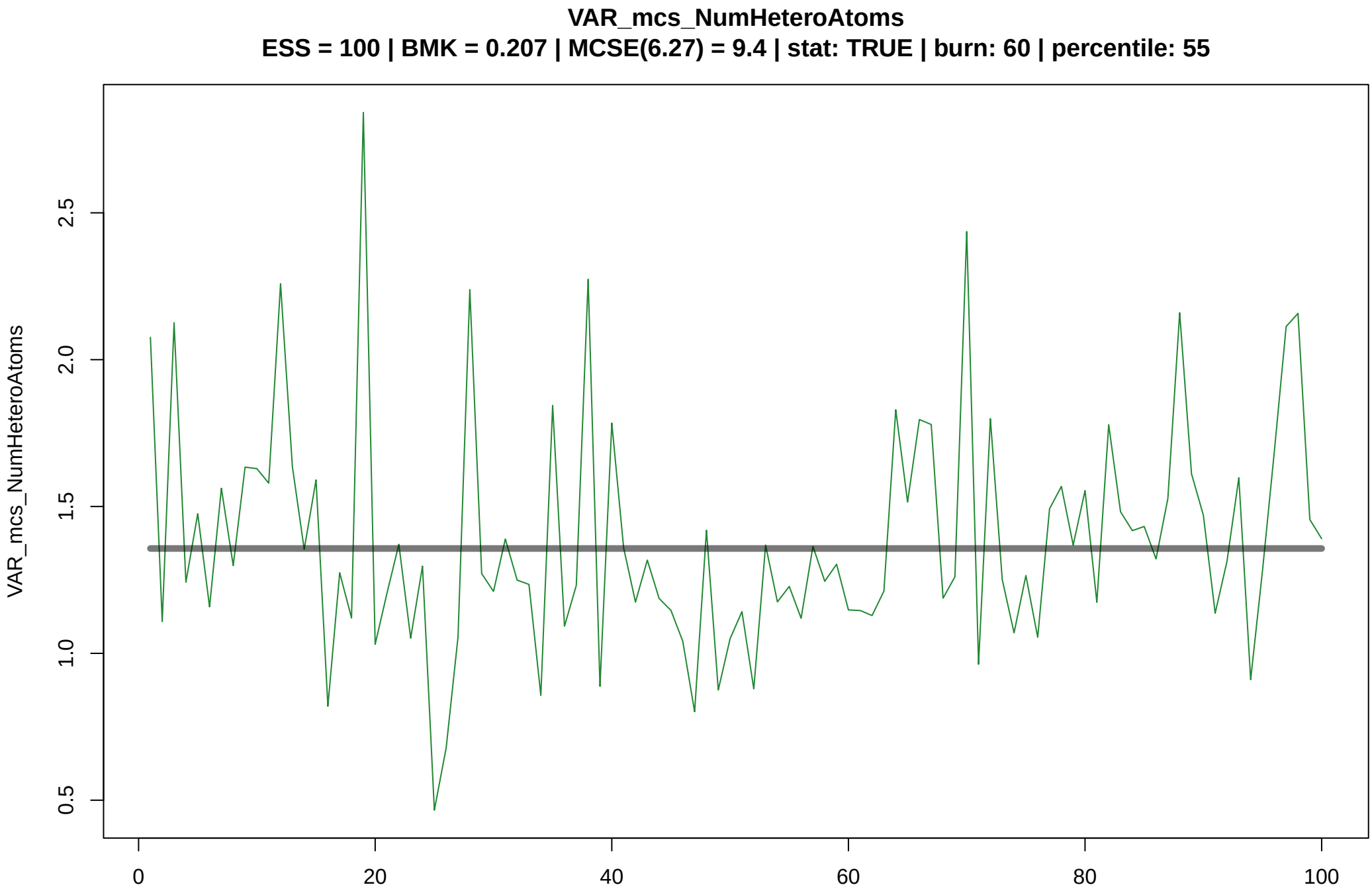

MEAN_docked_NumRotatableBonds
ESS = 100 | BMK = 0.175 | MCSE(6.27) = 10.4 | stat: FALSE | burn: 30 | percentile: 9
MEAN_docked_NumRotatableBonds
5
10
15
0
20
40
60
80
100

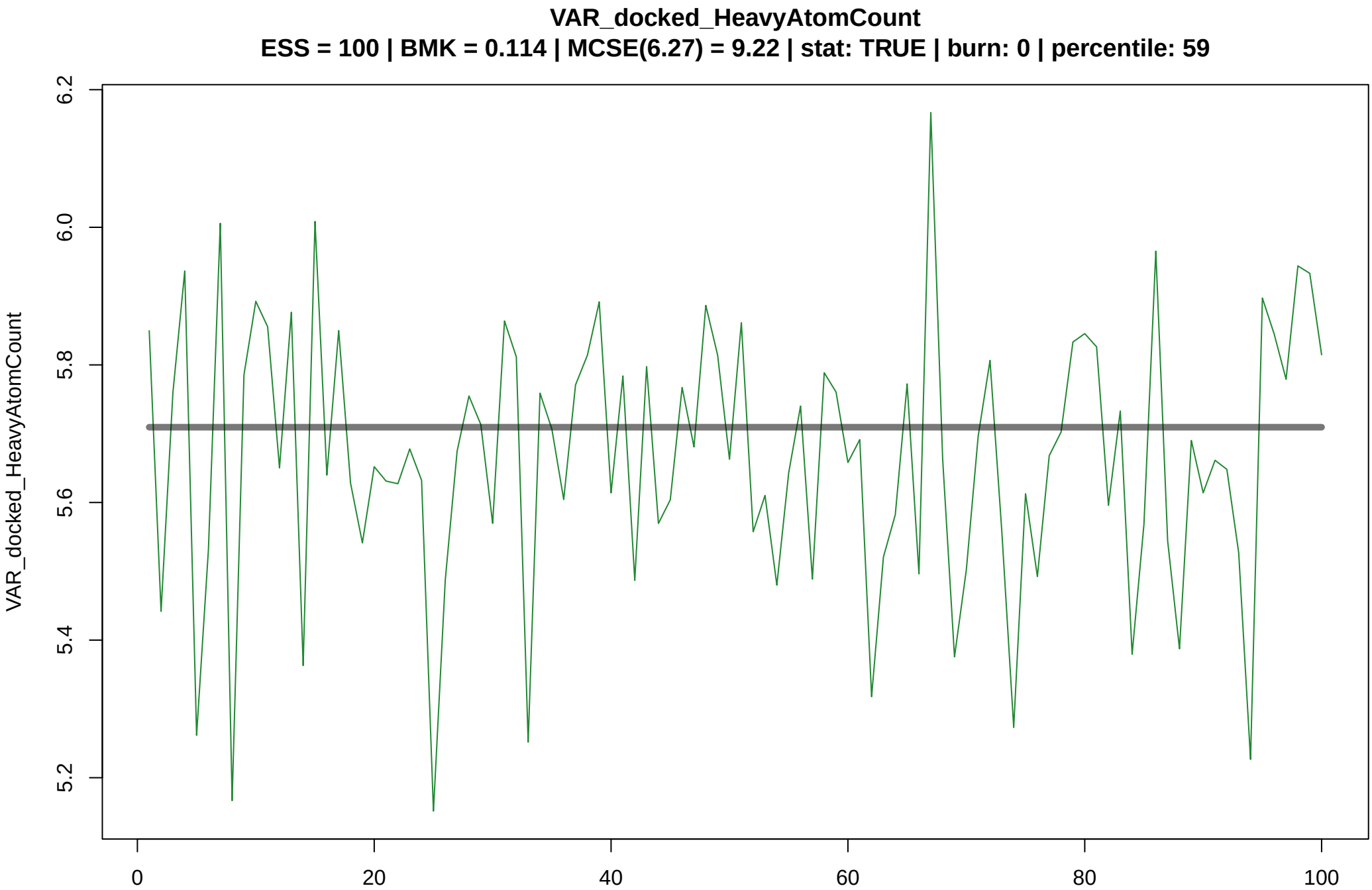

MEAN_mcs_NOCount
ESS = 70.6 | BMK = 0.181 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 0 | percentile: 3
MEAN_mcs_NOCount
10
15
20
0
20
40
60
80
100

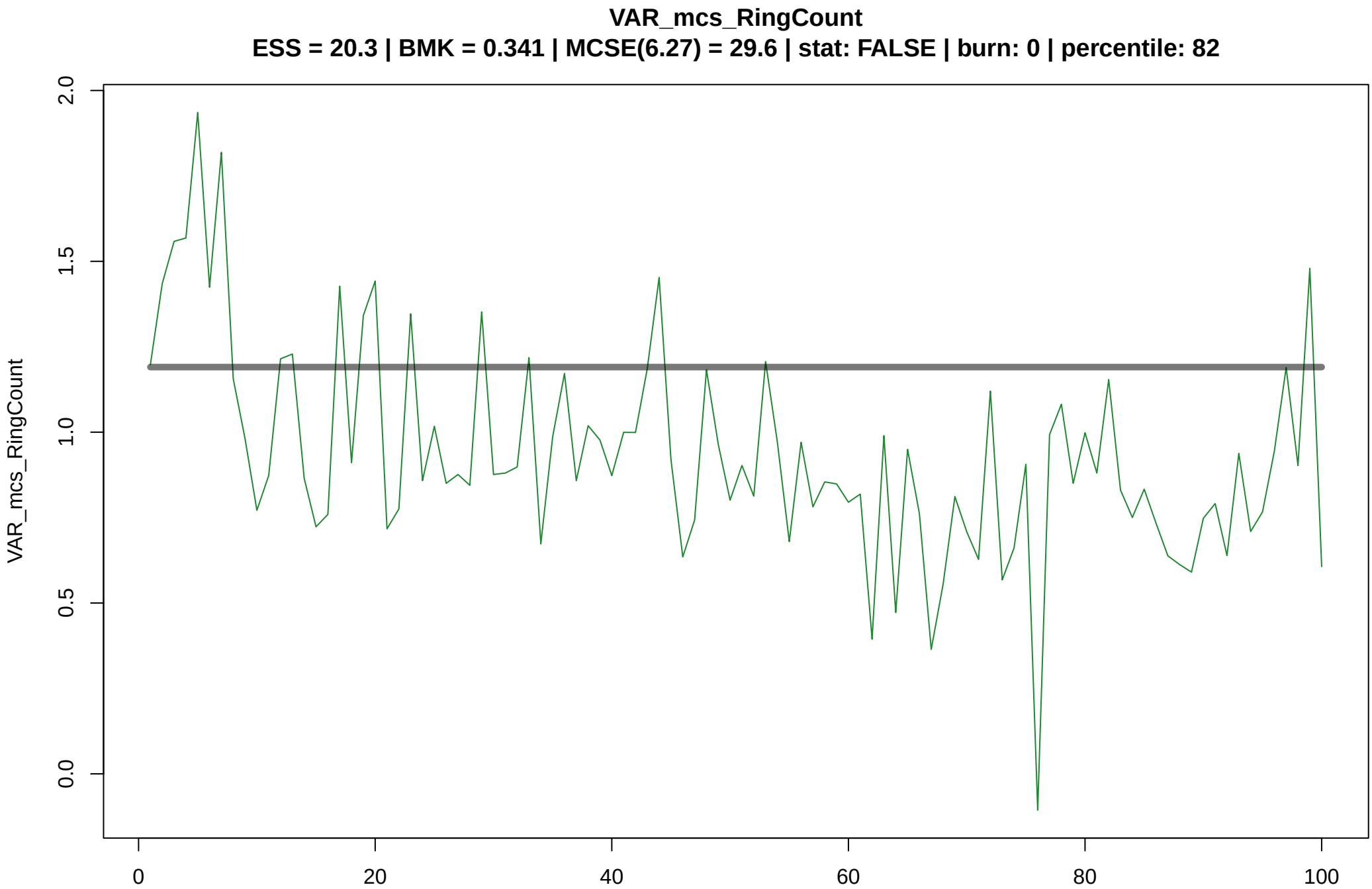

VAR_log_RMSD
ESS = 71.7 | BMK = 0.401 | MCSE(6.27) = 12.5 | stat: TRUE | burn: 80 | percentile: 26
VAR_log_RMSD
0
2
4
6
8
0
20
40
60
80
100

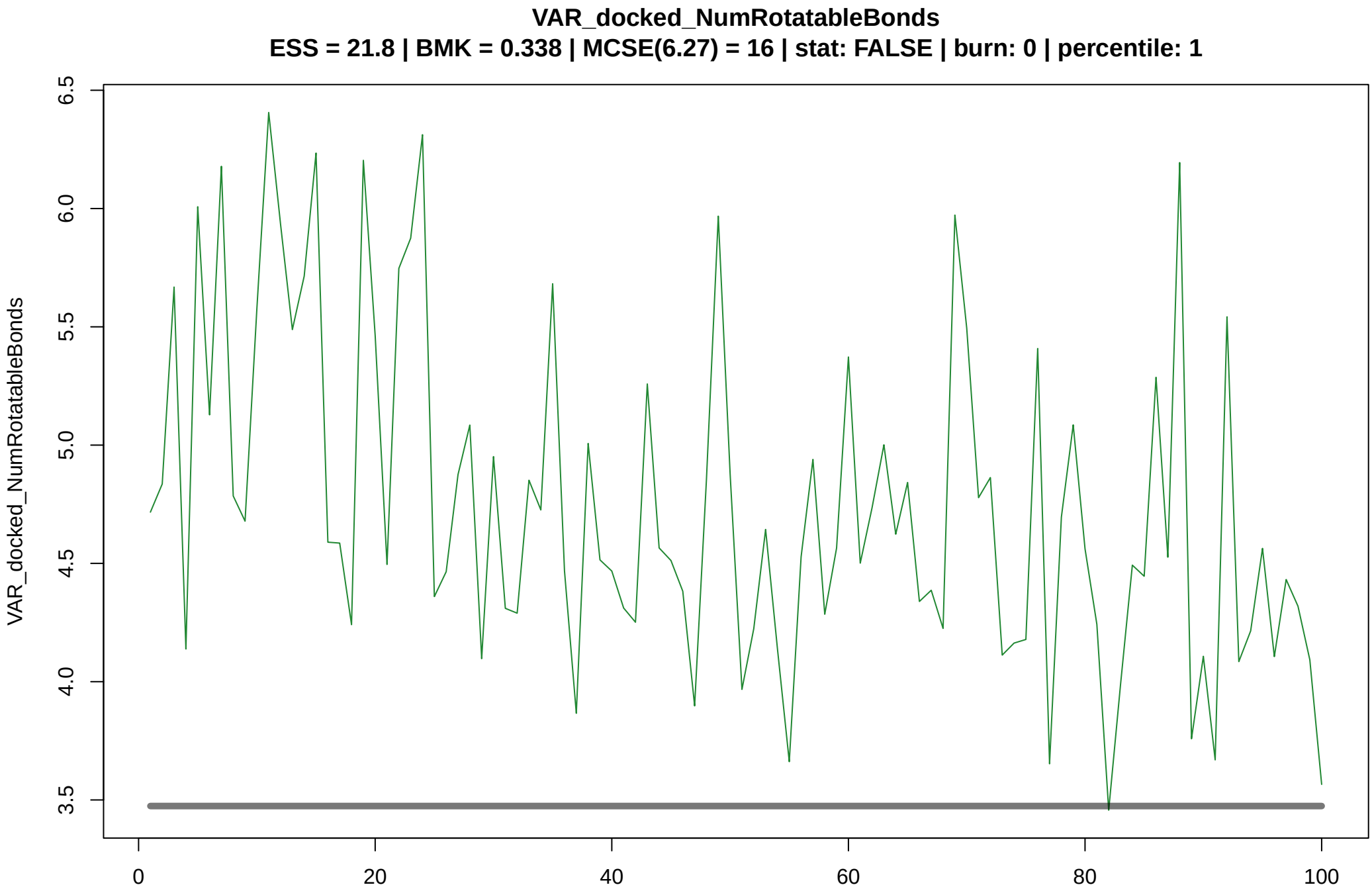

VAR_log_mcs_unbonded_polar_sasa
ESS = 100 | BMK = 1 | MCSE(6.27) = 9.74 | stat: TRUE | burn: 100 | percentile: 25
VAR_log_mcs_unbonded_polar_sasa
2
4
6
8
0
20
40
60
80
100

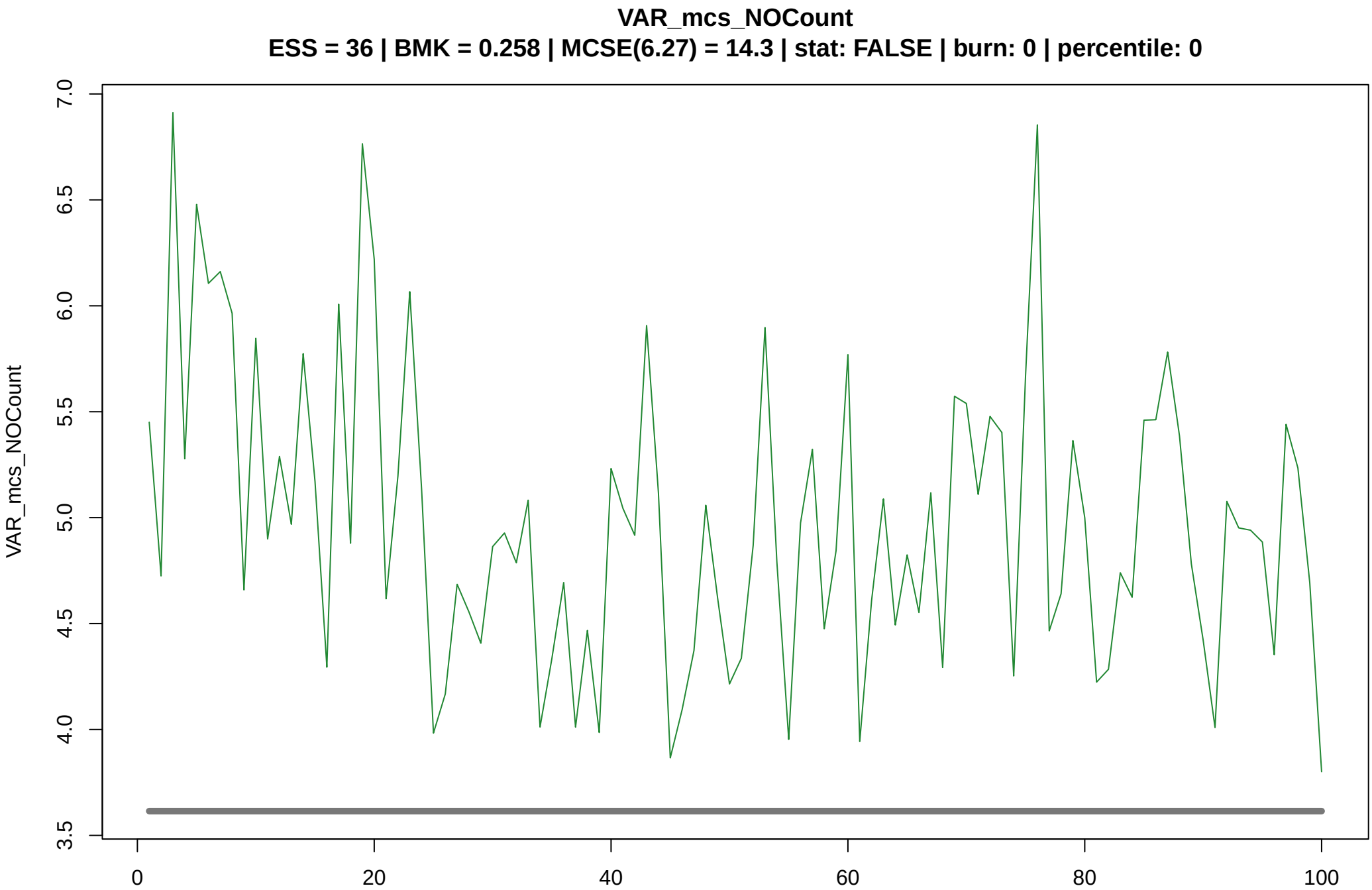

VAR_logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.283 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 70 | percentile: 41
VAR_logit_ec_tanimoto_similarity
2
3
4
5
6
7
8
0
20
40
60
80
100

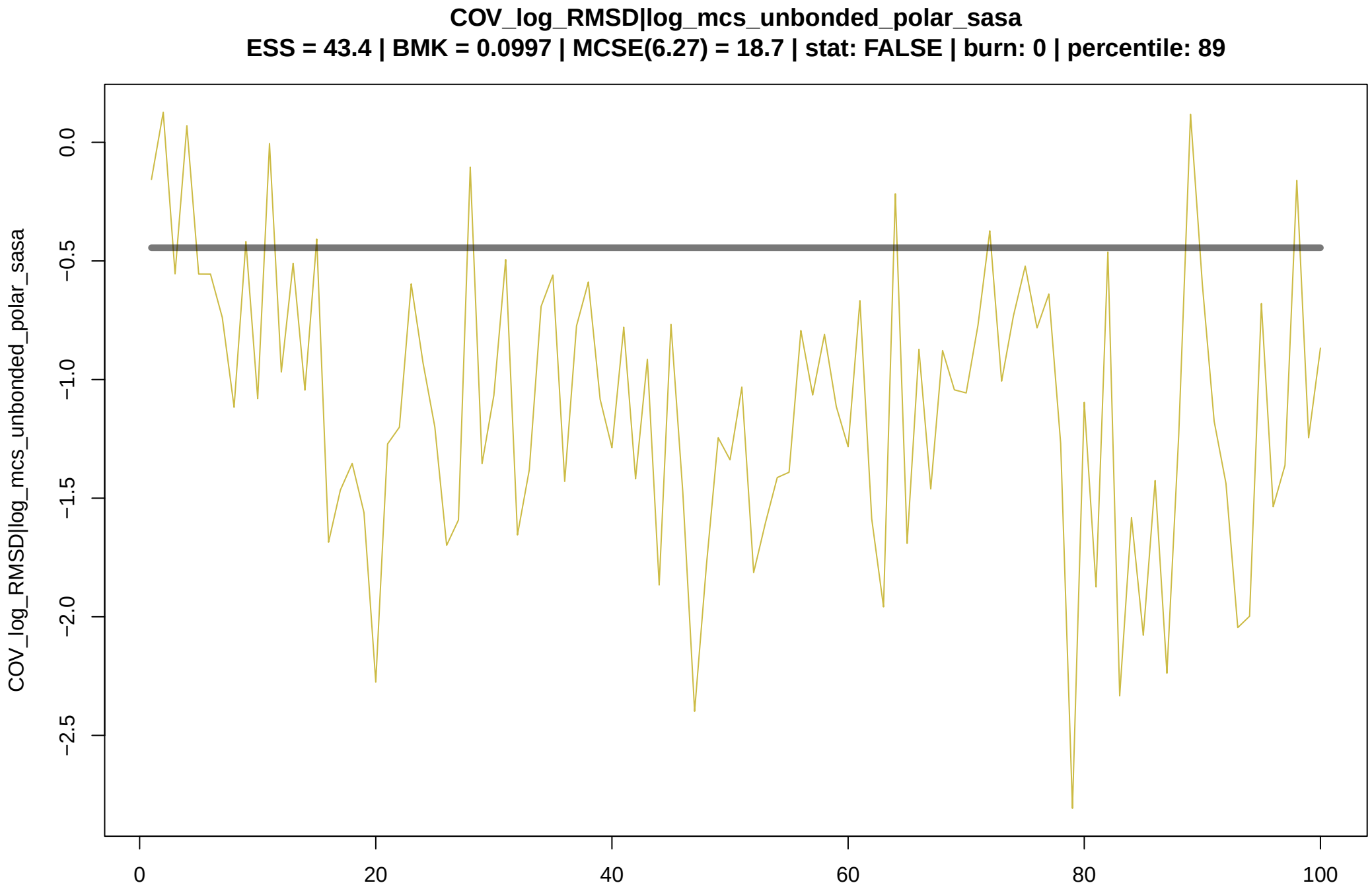

VAR_mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.207 | MCSE(6.27) = 9.4 | stat: TRUE | burn: 60 | percentile: 55
VAR_mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100

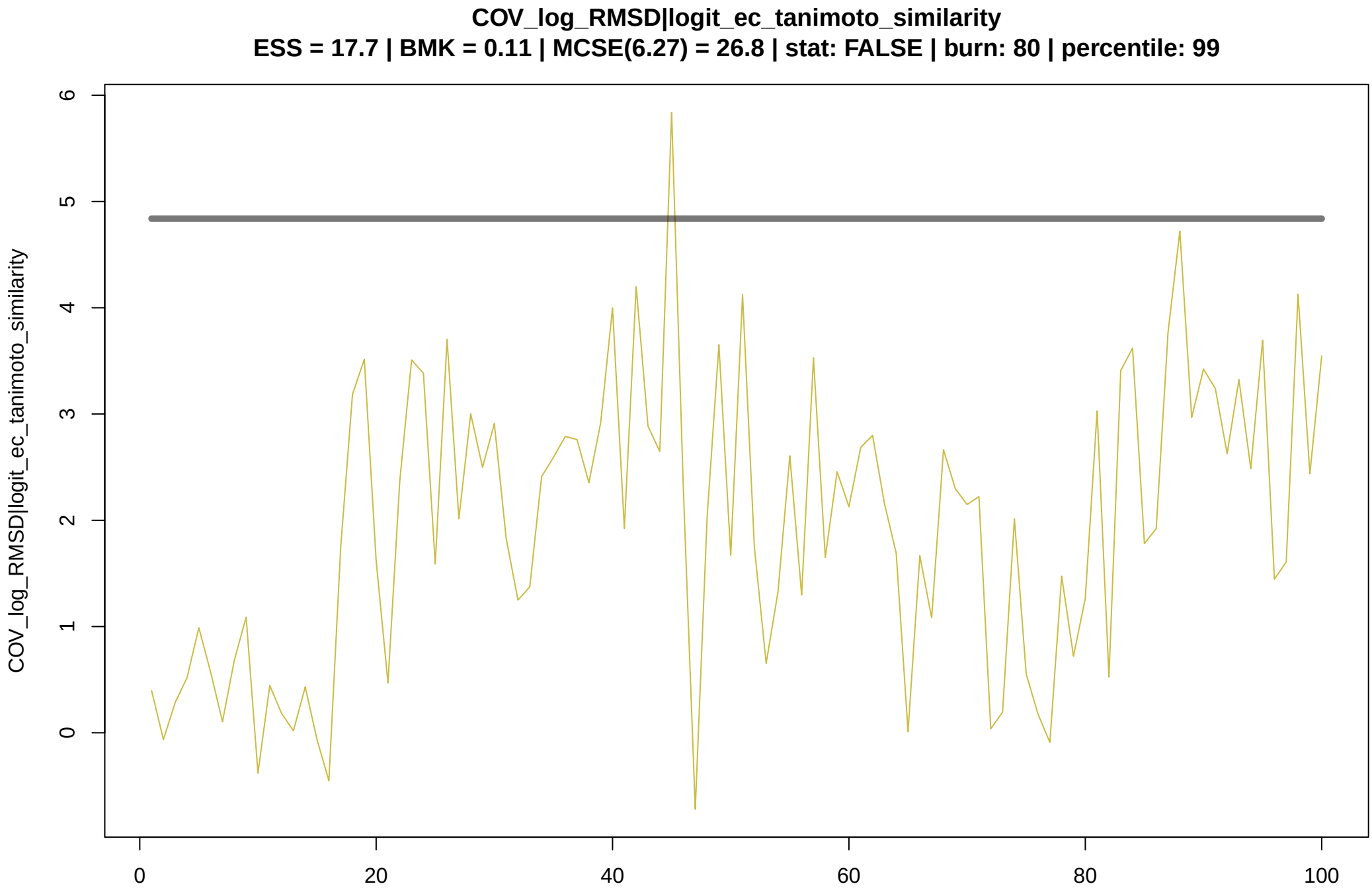

VAR_docked_HeavyAtomCount
ESS = 100 | BMK = 0.114 | MCSE(6.27) = 9.22 | stat: TRUE | burn: 0 | percentile: 59
VAR_docked_HeavyAtomCount
6.2
6.0
5.8
5.6
5.4
5.2
0
20
40
60
80
100

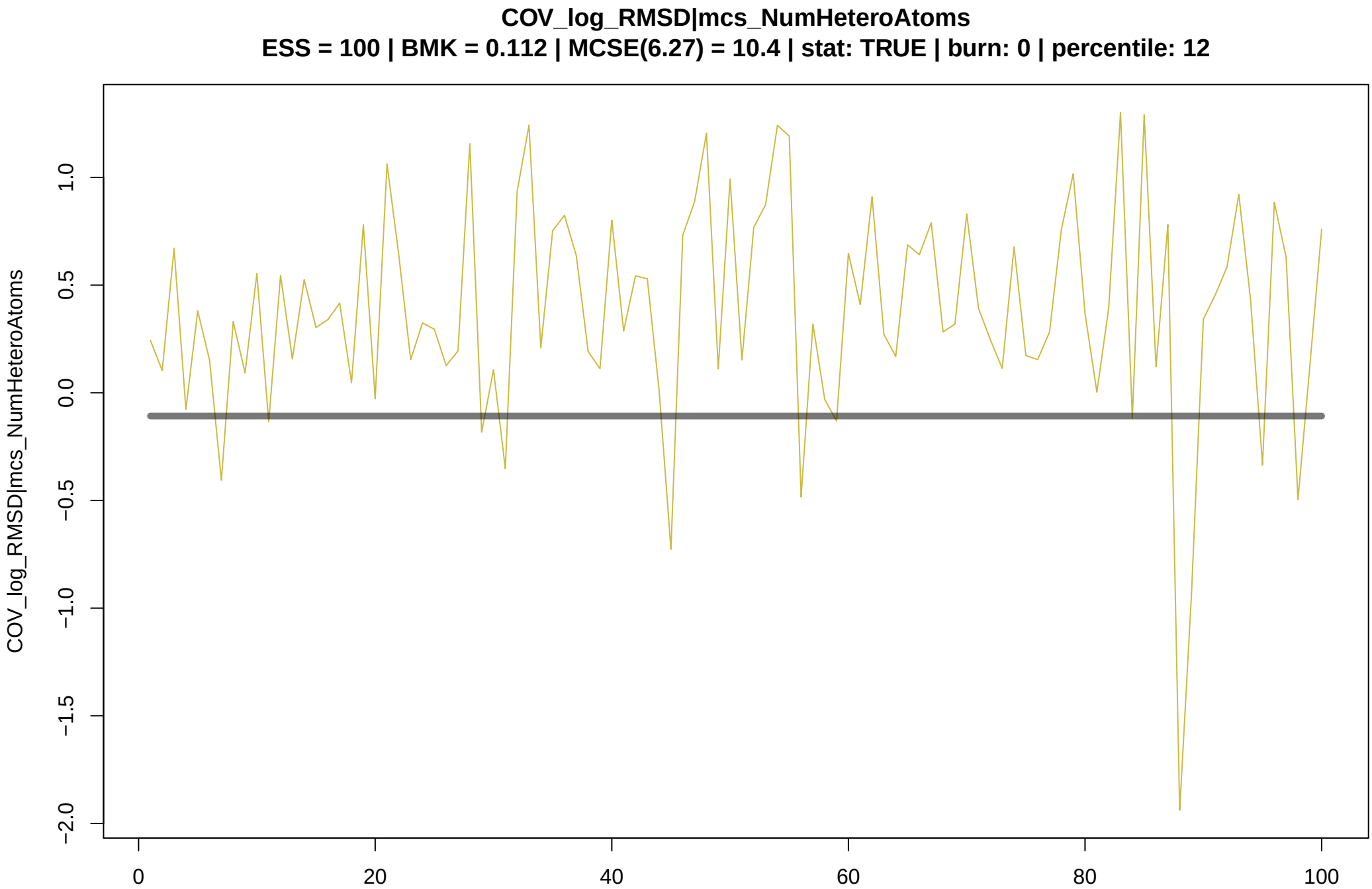

VAR_mcs_RingCount
ESS = 20.3 | BMK = 0.341 | MCSE(6.27) = 29.6 | stat: FALSE | burn: 0 | percentile: 82
VAR_mcs_RingCount
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100

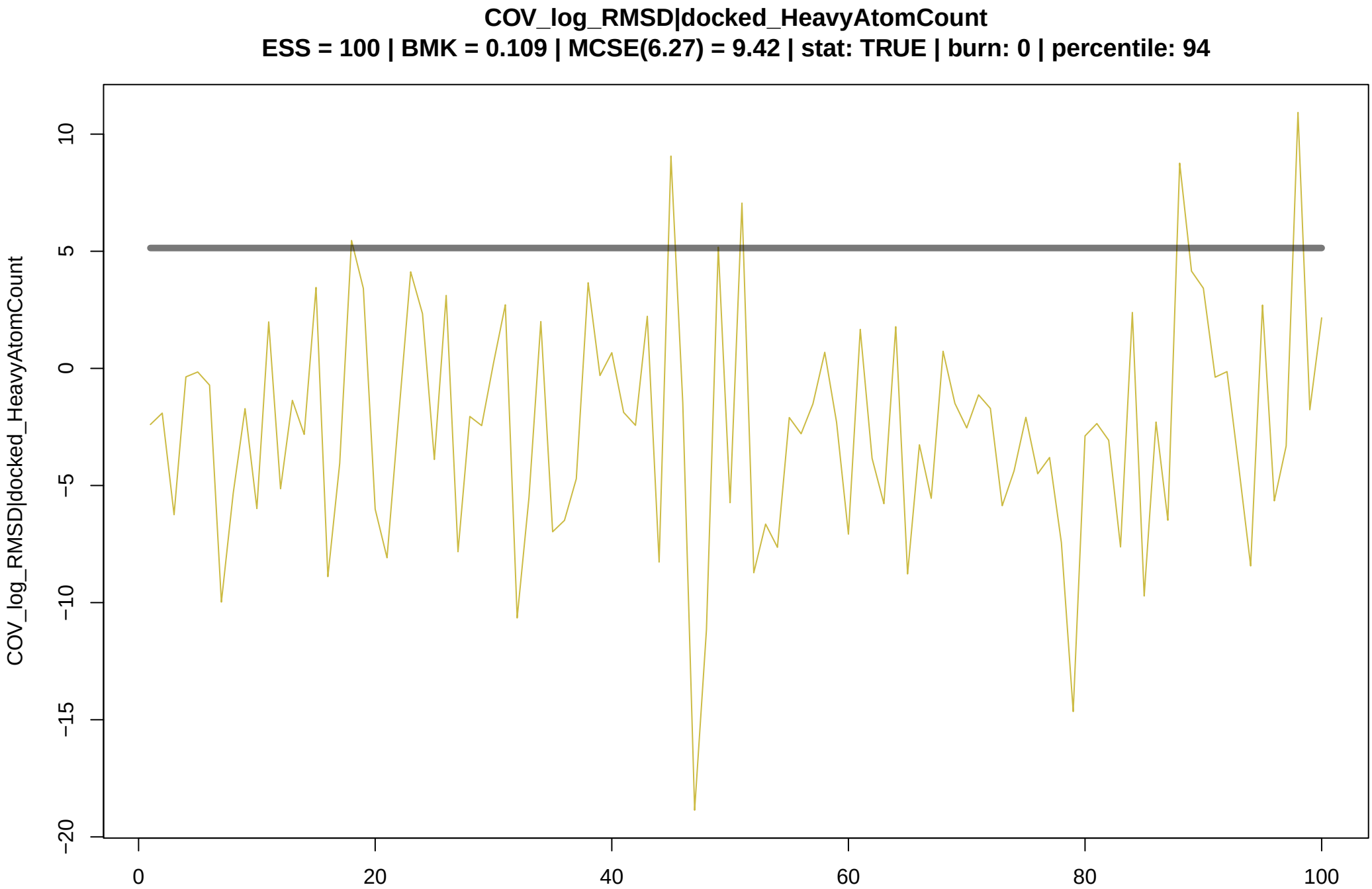

VAR_docked_NumRotatableBonds
ESS = 21.8 | BMK = 0.338 | MCSE(6.27) = 16 | stat: FALSE | burn: 0 | percentile: 1
VAR_docked_NumRotatableBonds
3.5
4.0
4.5
5.0
5.5
6.0
6.5
0
20
40
60
80
100

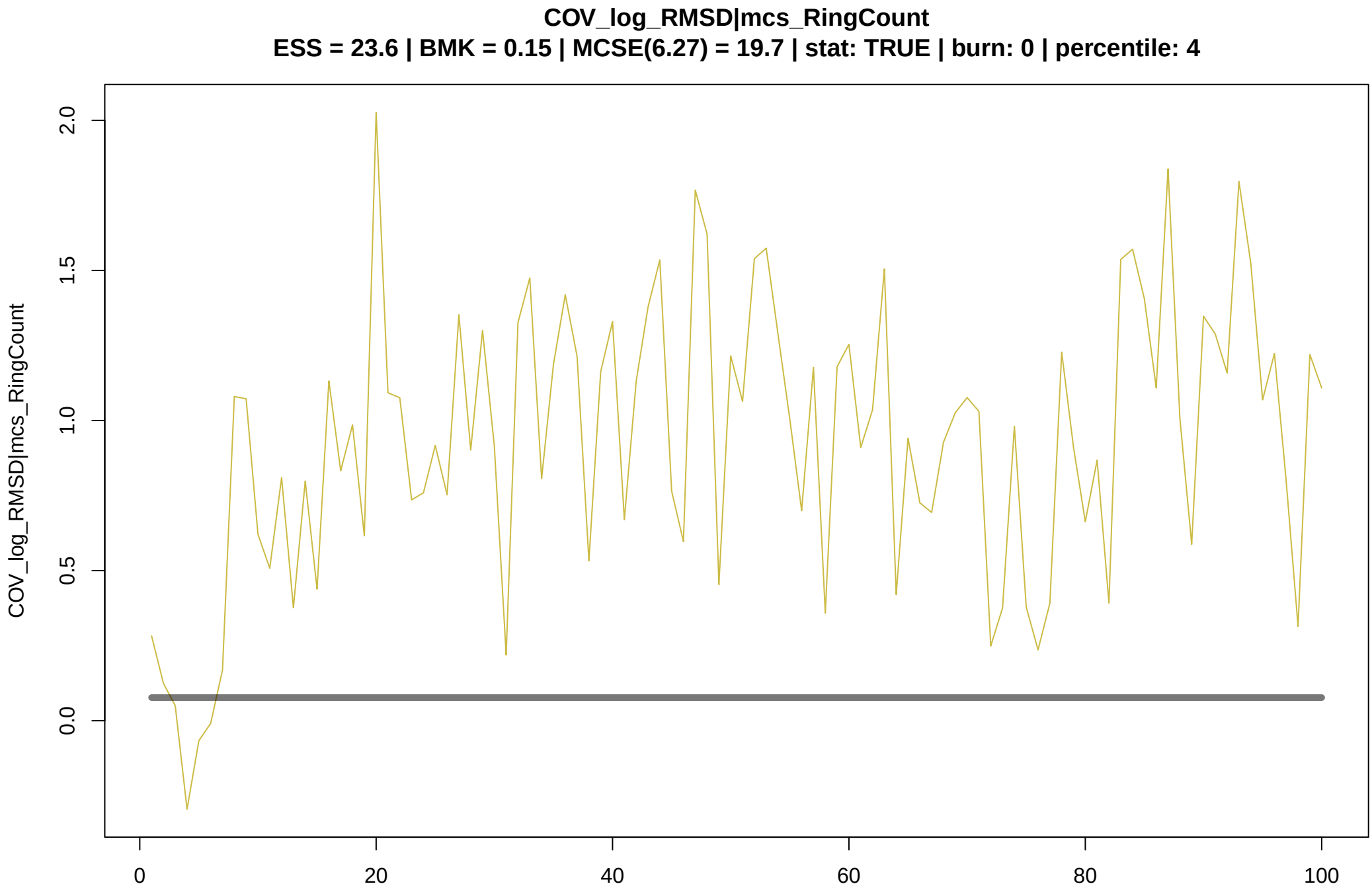

VAR_mcs_NOCount
ESS = 36 | BMK = 0.258 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 0 | percentile: 0
VAR_mcs_NOCount
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
0
20
40
60
80
100

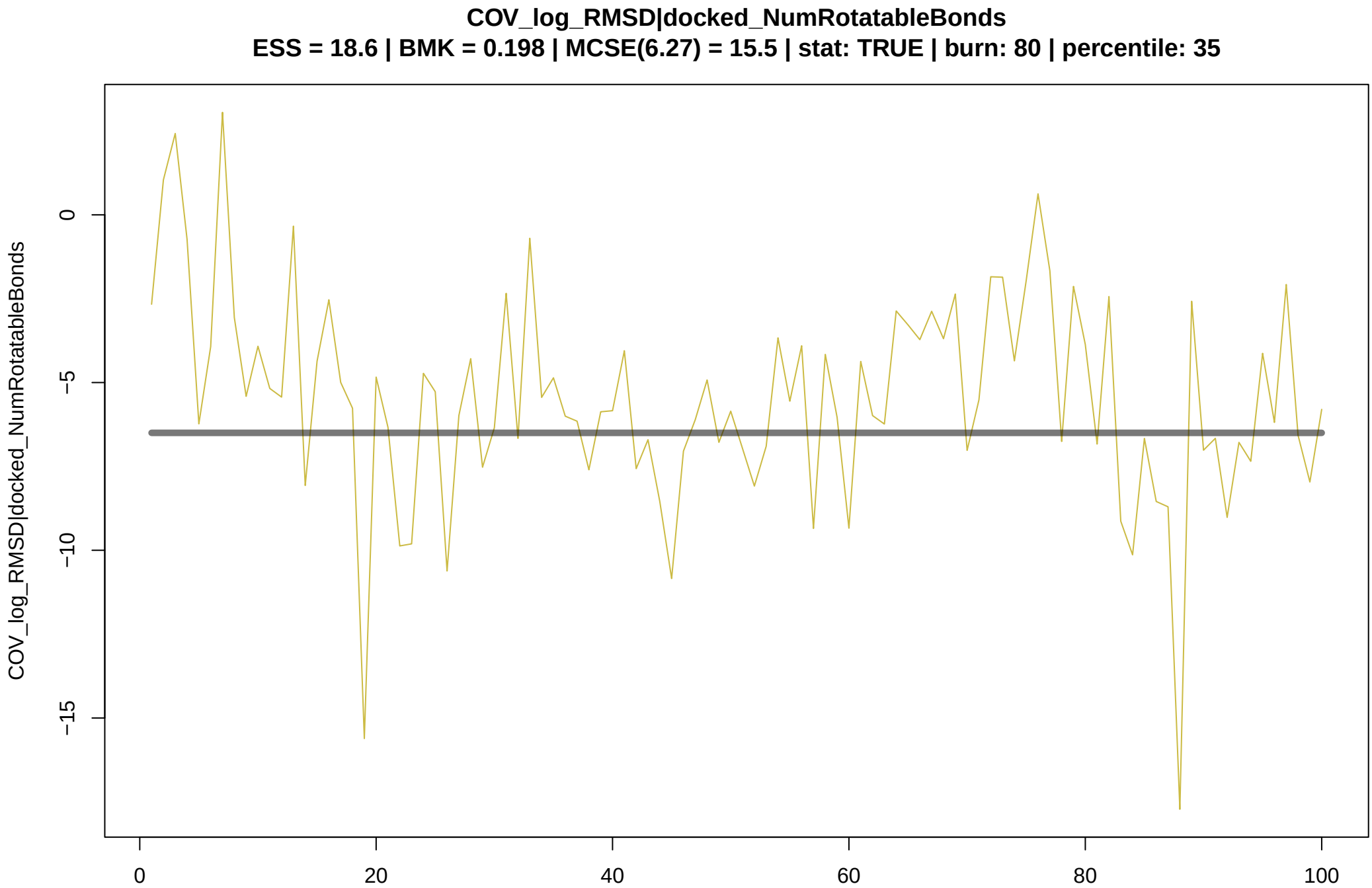

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 43.4 | BMK = 0.0997 | MCSE(6.27) = 18.7 | stat: FALSE | burn: 0 | percentile: 89
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
20
40
60
80
100

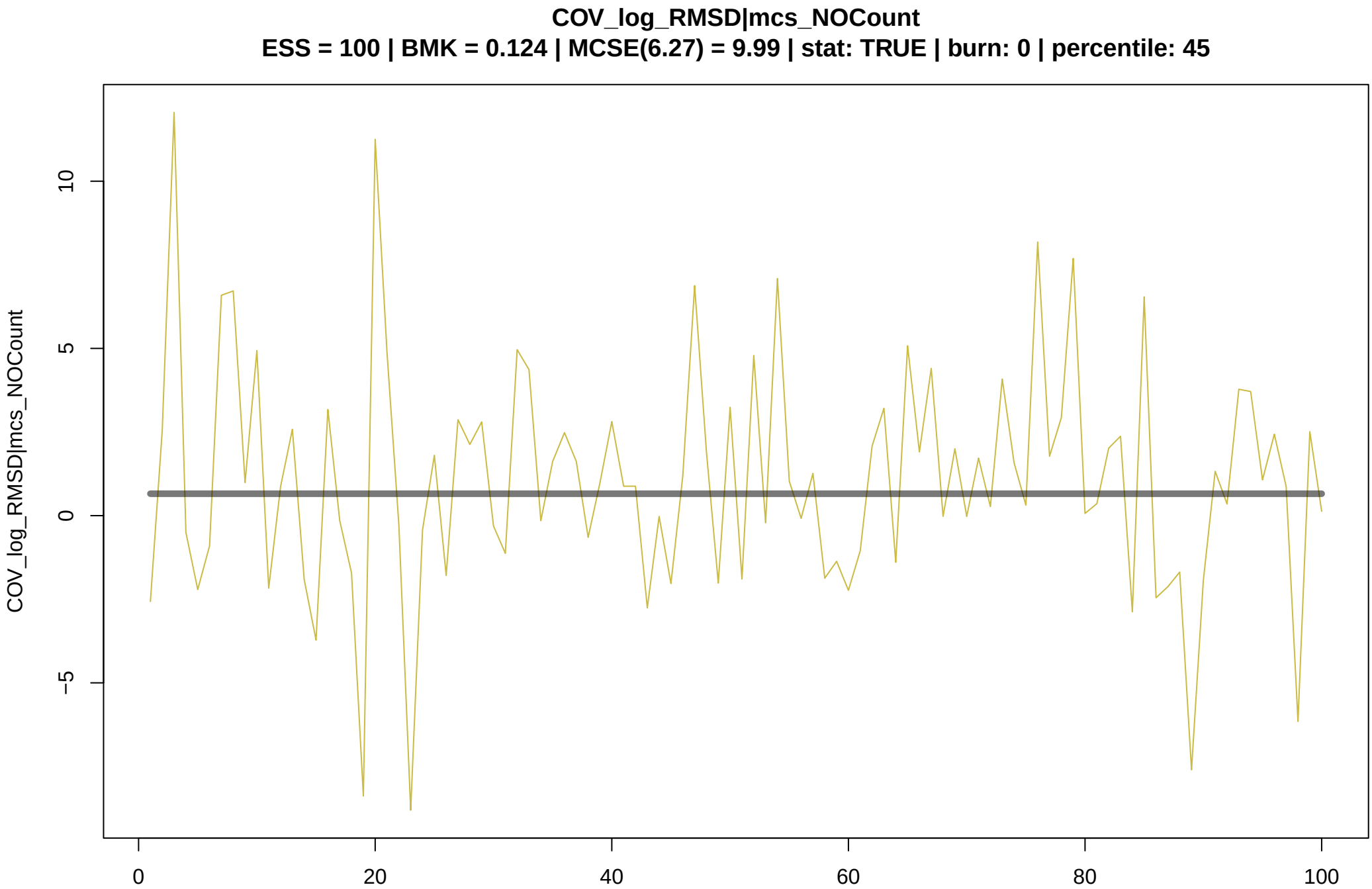

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 17.7 | BMK = 0.11 | MCSE(6.27) = 26.8 | stat: FALSE | burn: 80 | percentile: 99
COV_log_RMSD|logit_ec_tanimoto_similarity
0
1
2
3
4
5
6
0
20
40
60
80
100

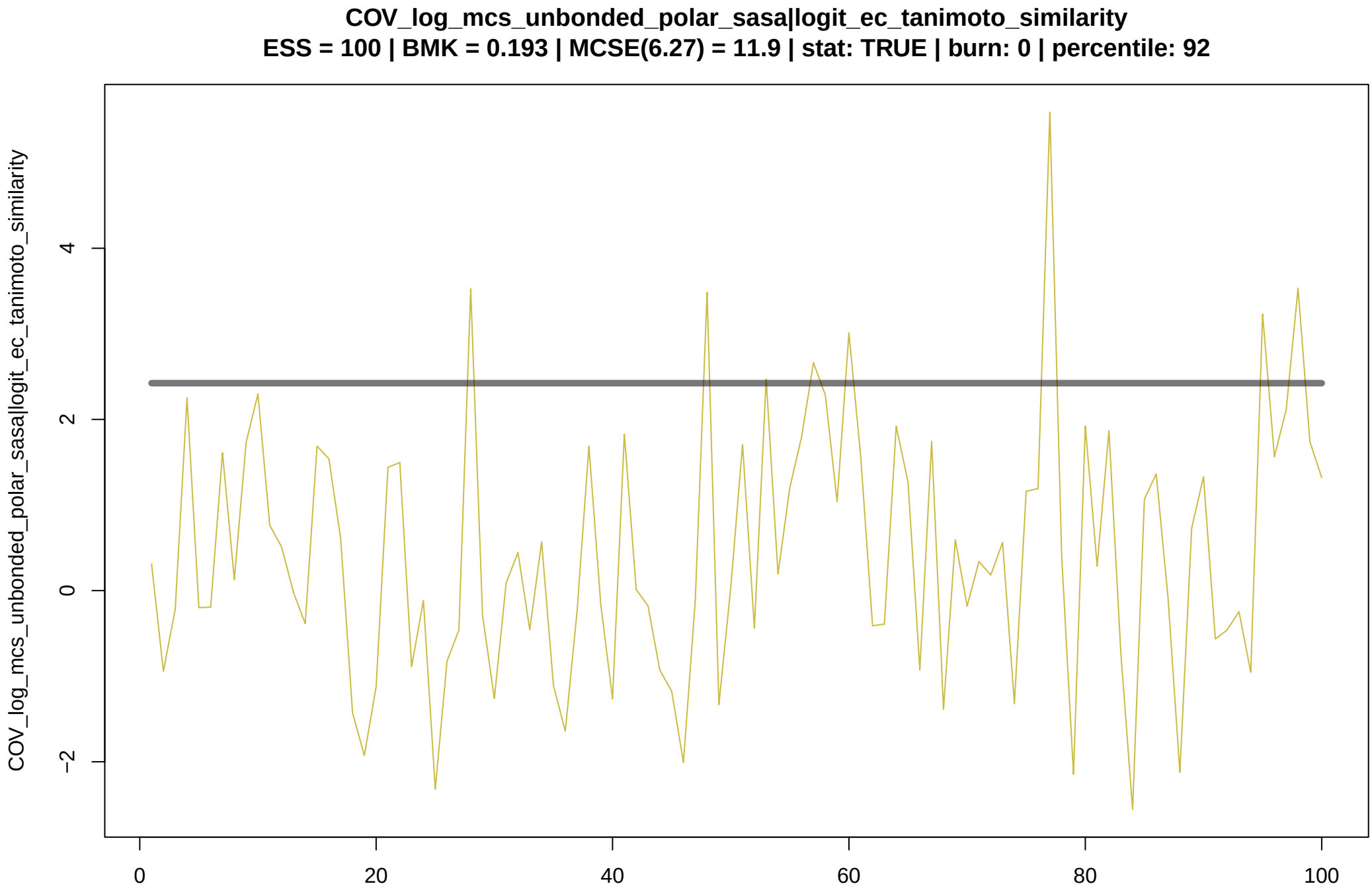

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.112 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 0 | percentile: 12
COV_log_RMSD|mcs_NumHeteroAtoms
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
20
40
60
80
100

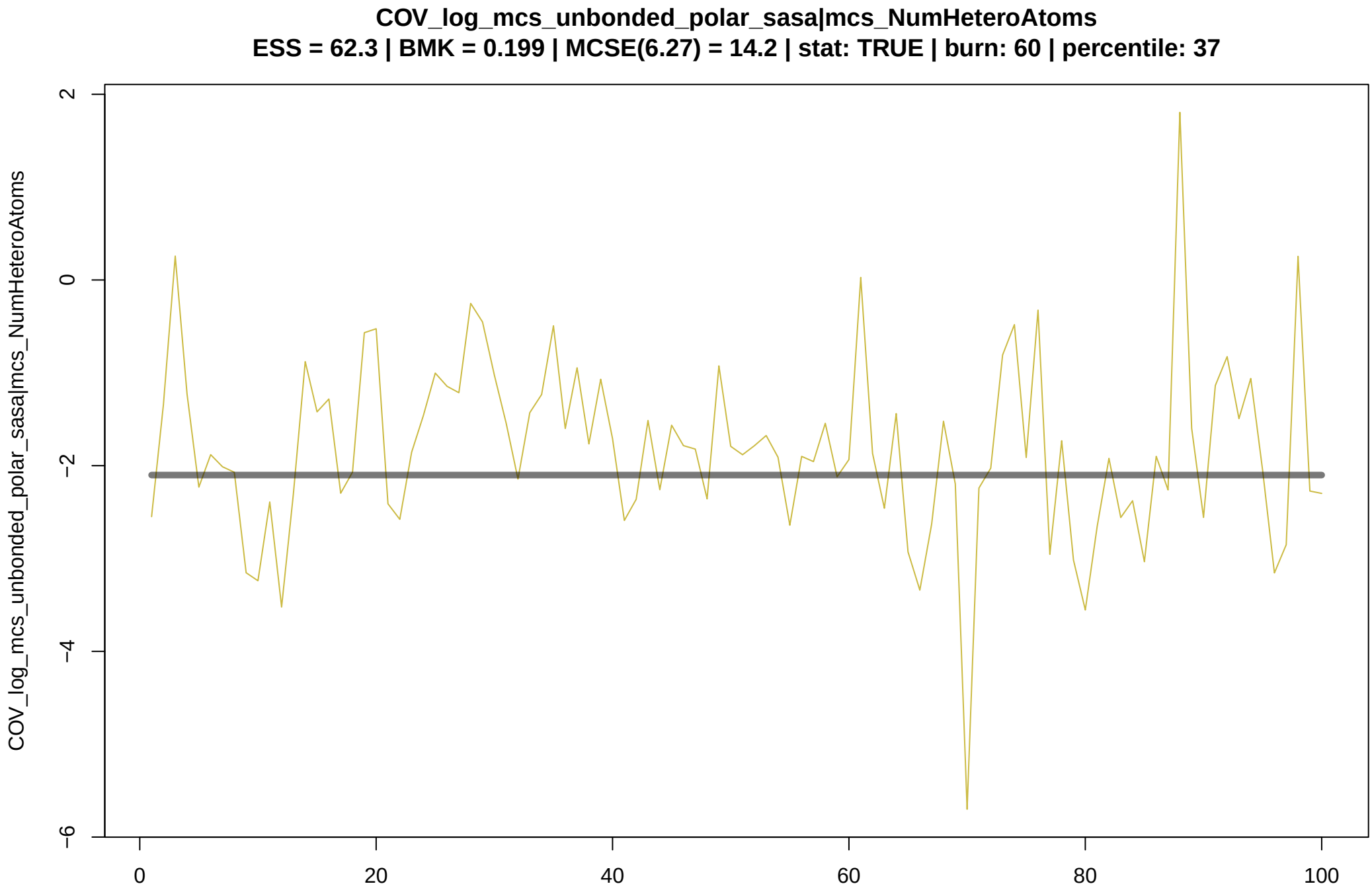

COV_log_RMSD|docked_HeavyAtomCount
ESS = 100 | BMK = 0.109 | MCSE(6.27) = 9.42 | stat: TRUE | burn: 0 | percentile: 94
COV_log_RMSD|docked_HeavyAtomCount
10
5
0
−5
−10
−15
−20
0
20
40
60
80
100

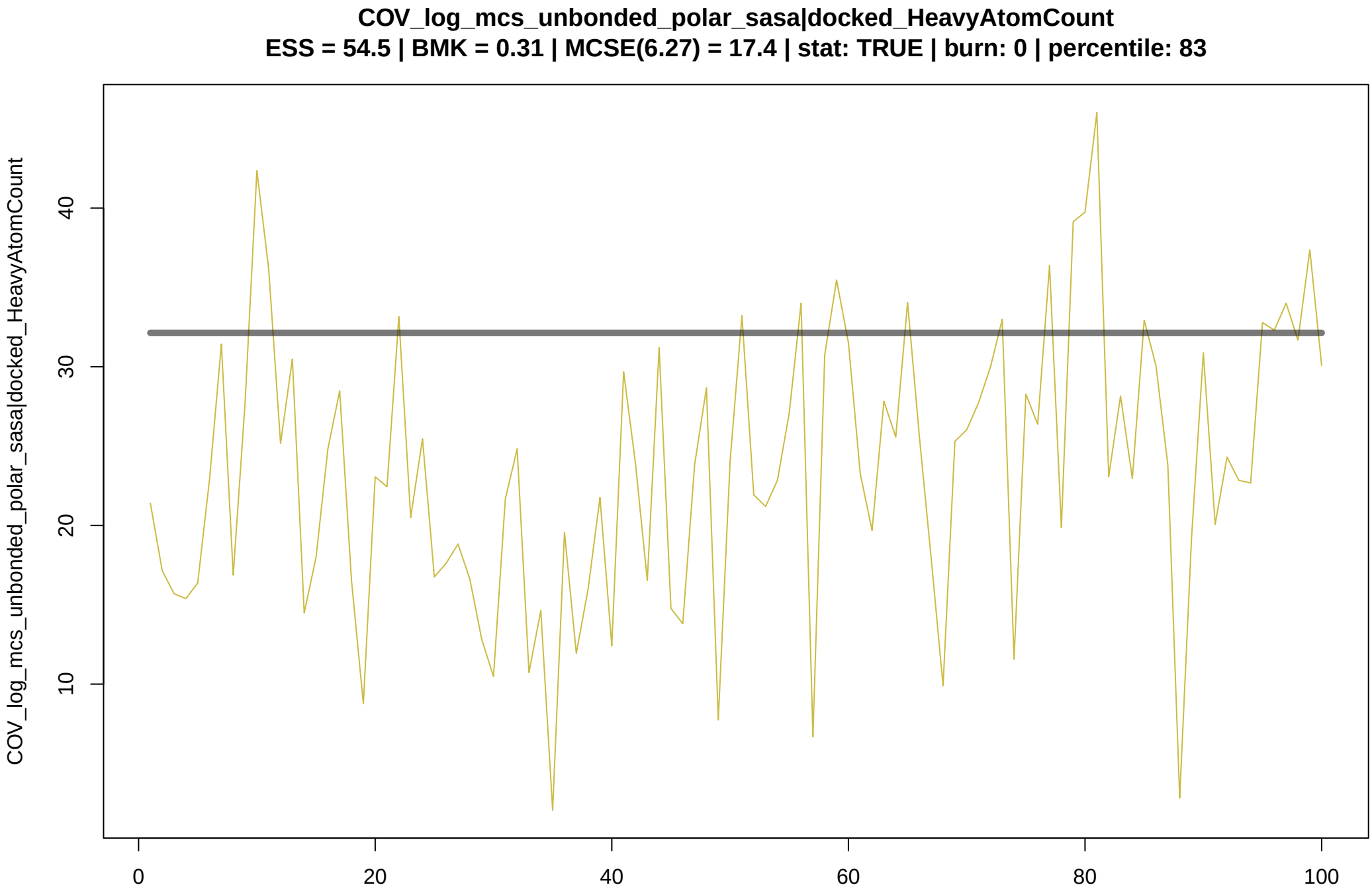

COV_log_RMSD|mcs_RingCount
ESS = 23.6 | BMK = 0.15 | MCSE(6.27) = 19.7 | stat: TRUE | burn: 0 | percentile: 4
COV_log_RMSD|mcs_RingCount
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100

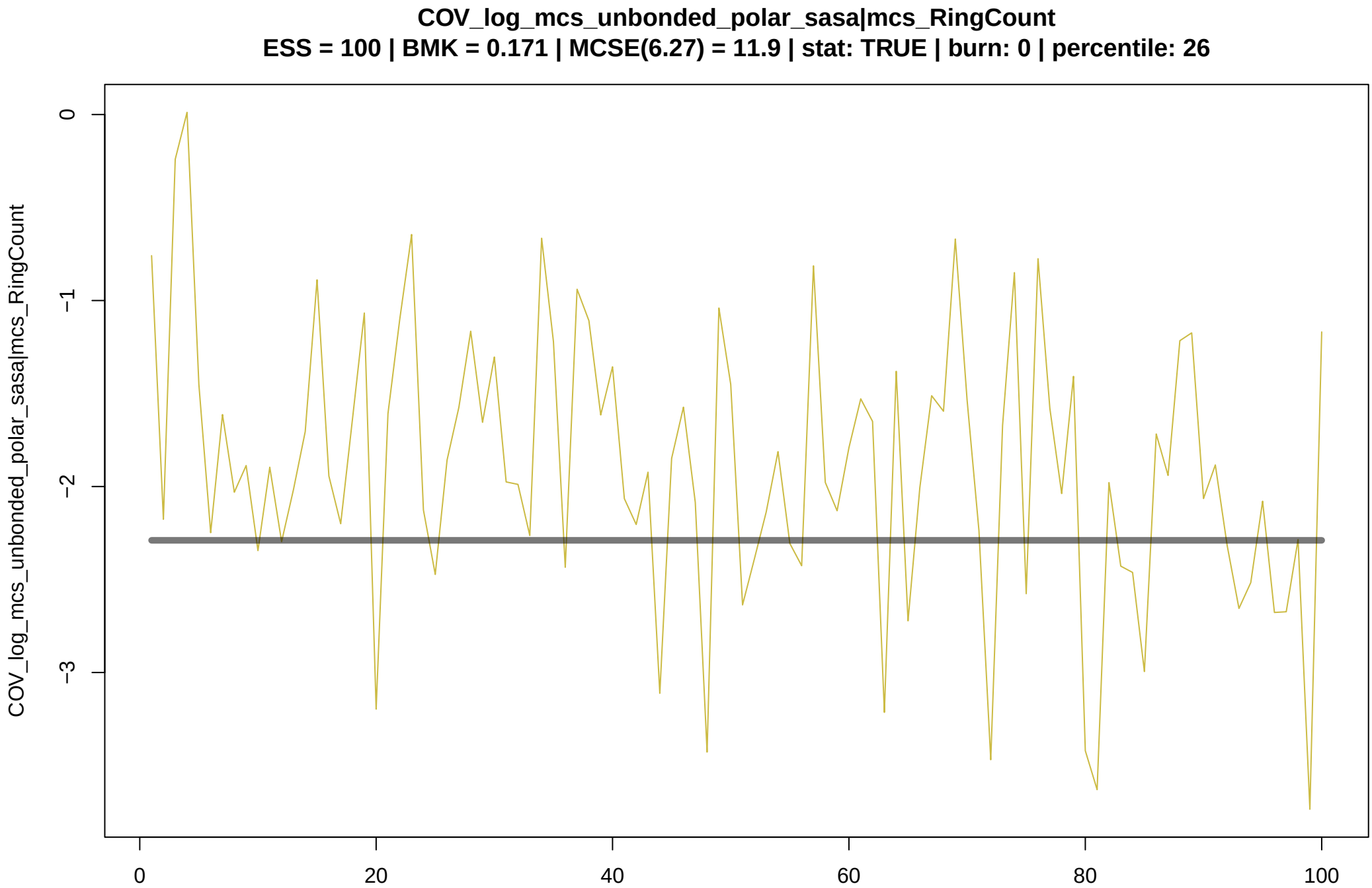

COV_log_RMSD|docked_NumRotatableBonds
ESS = 18.6 | BMK = 0.198 | MCSE(6.27) = 15.5 | stat: TRUE | burn: 80 | percentile: 35
COV_log_RMSD|docked_NumRotatableBonds
0
−5
−10
−15
0
20
40
60
80
100

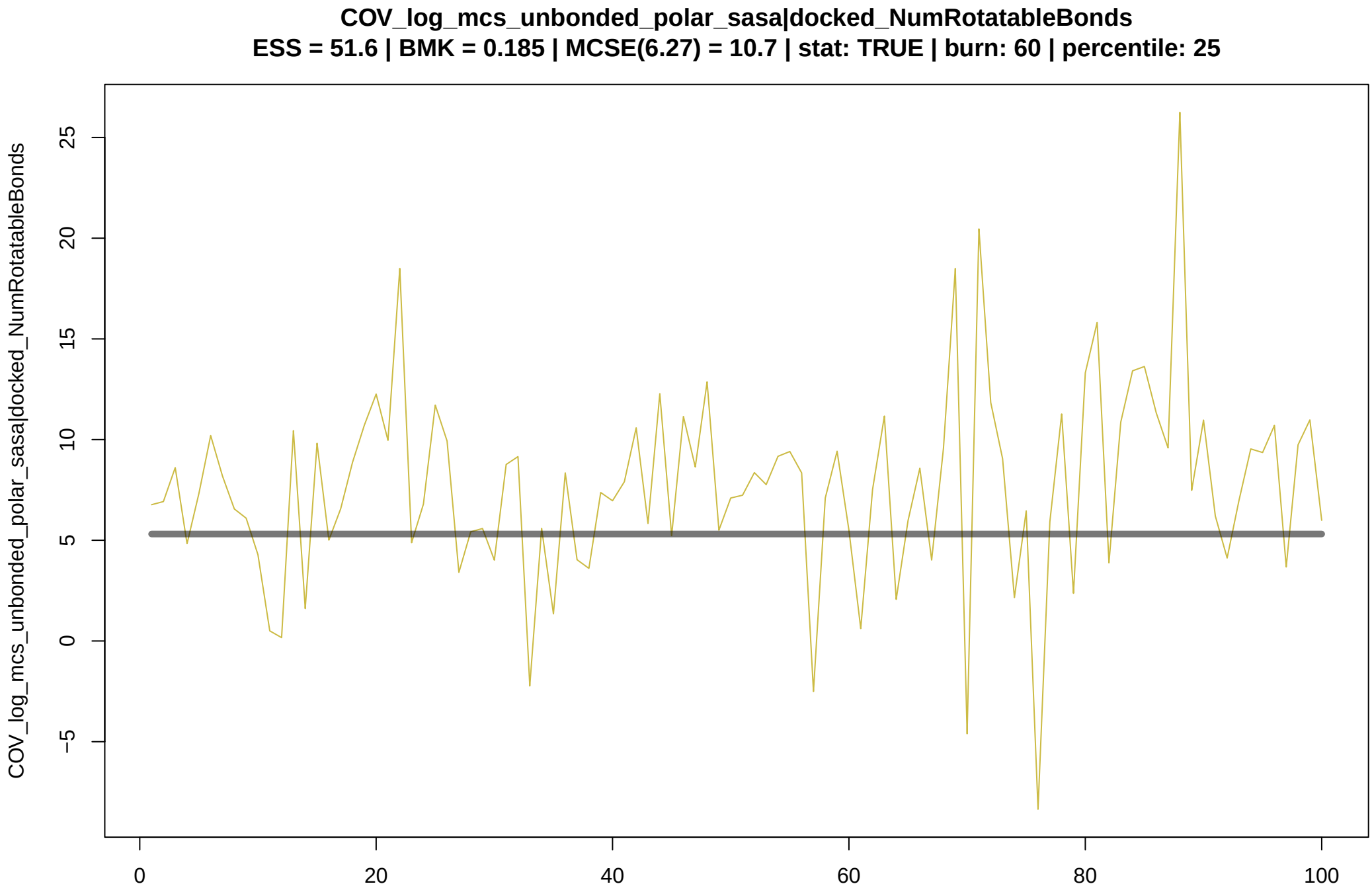

COV_log_RMSD|mcs_NOCount
ESS = 100 | BMK = 0.124 | MCSE(6.27) = 9.99 | stat: TRUE | burn: 0 | percentile: 45
COV_log_RMSD|mcs_NOCount
10
5
0
−5
0
20
40
60
80
100

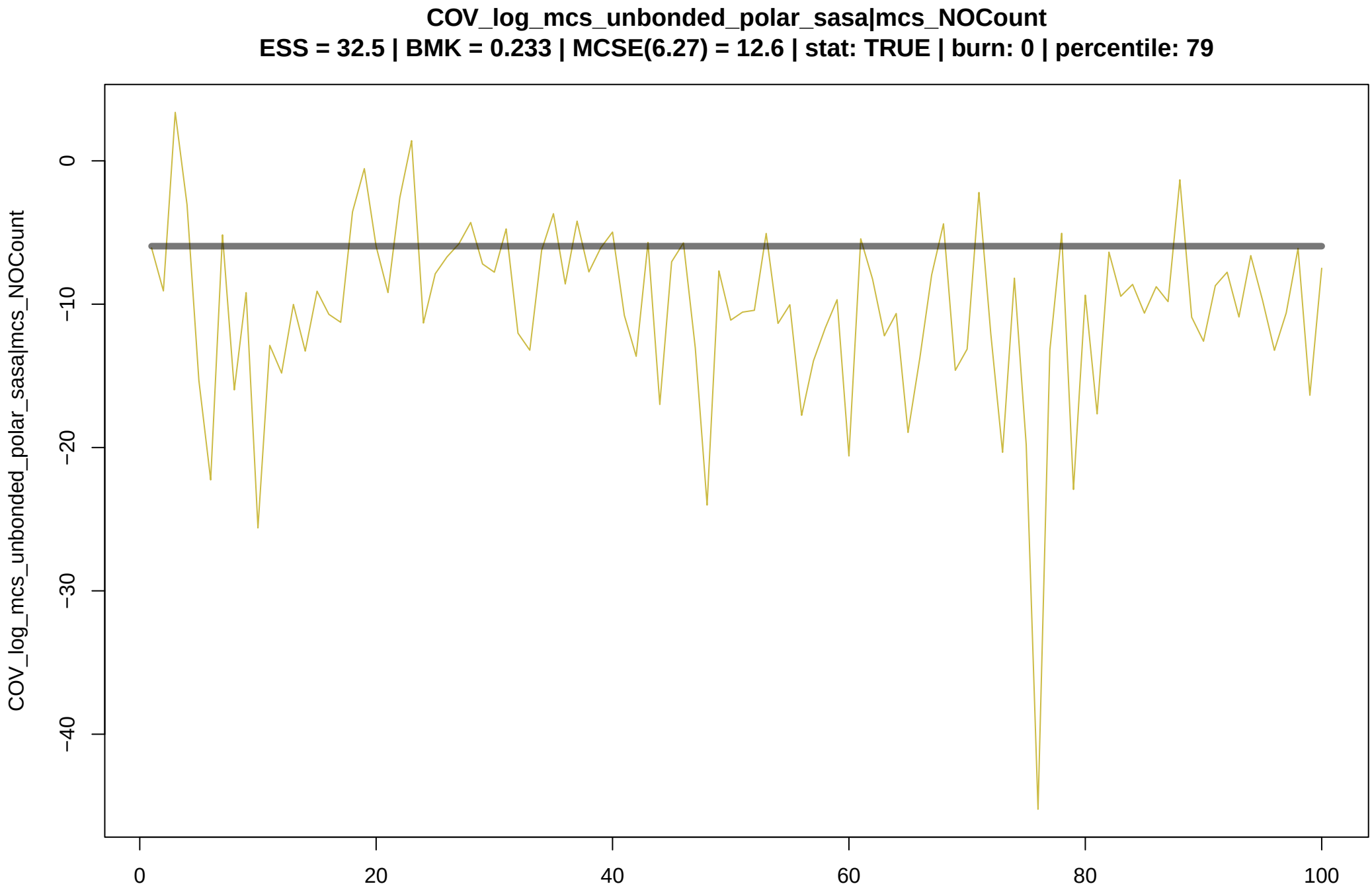

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 100 | BMK = 0.193 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 0 | percentile: 92
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
4
2
0
−2
0
20
40
60
80
100

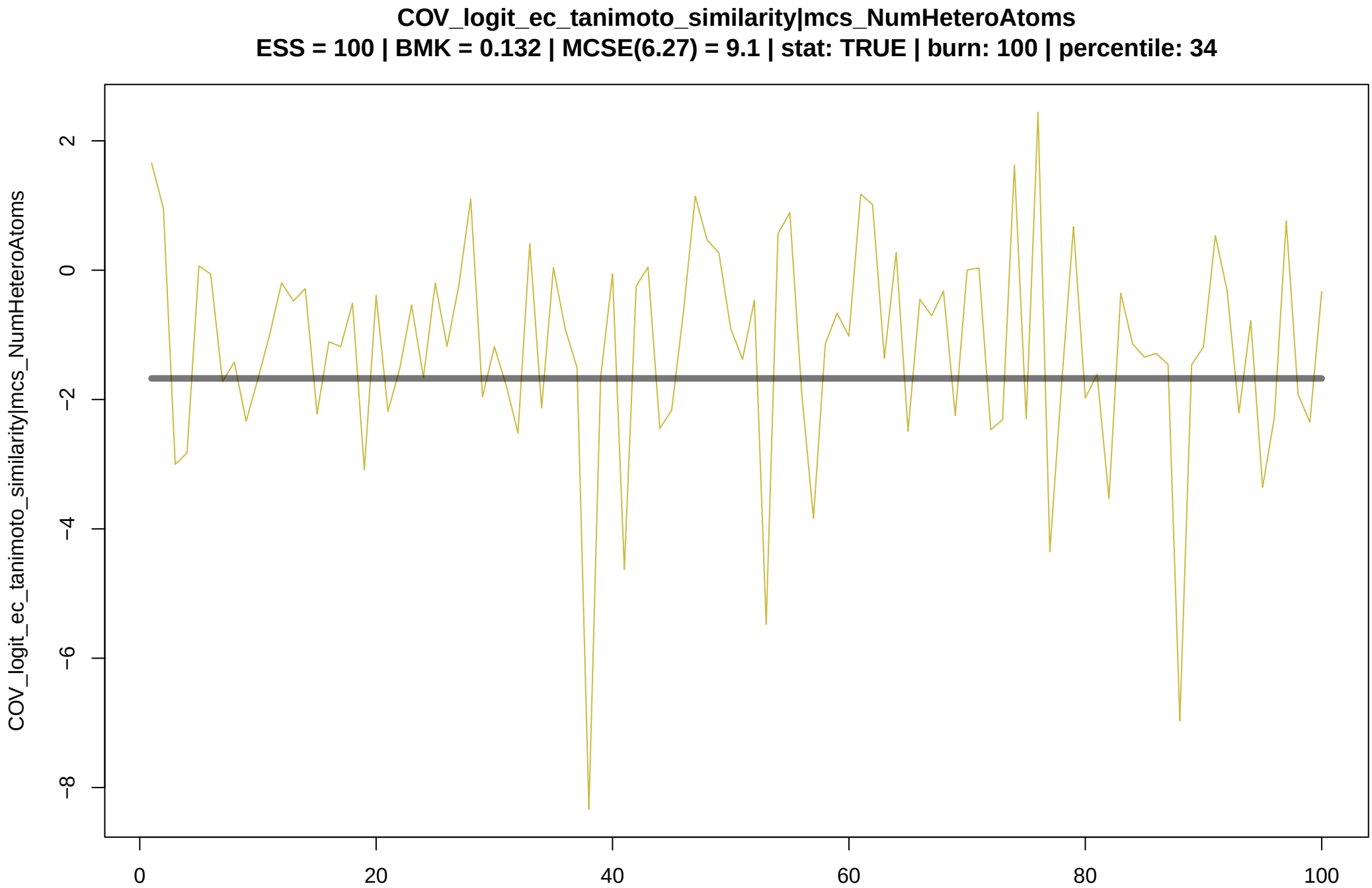

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 62.3 | BMK = 0.199 | MCSE(6.27) = 14.2 | stat: TRUE | burn: 60 | percentile: 37
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
2
0
−2
−4
−6
0
20
40
60
80
100

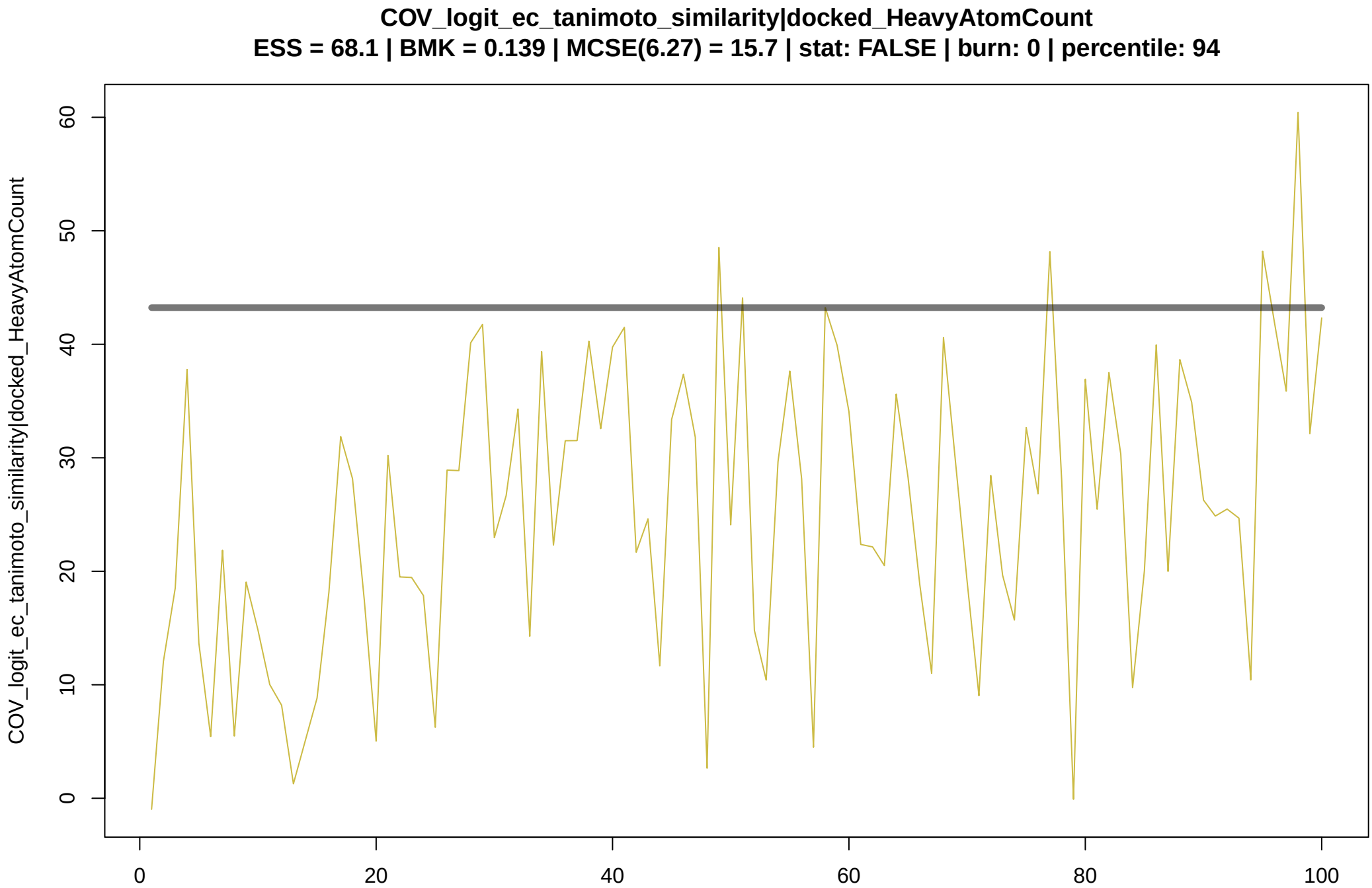

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 54.5 | BMK = 0.31 | MCSE(6.27) = 17.4 | stat: TRUE | burn: 0 | percentile: 83
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
10
20
30
40
0
20
40
60
80
100

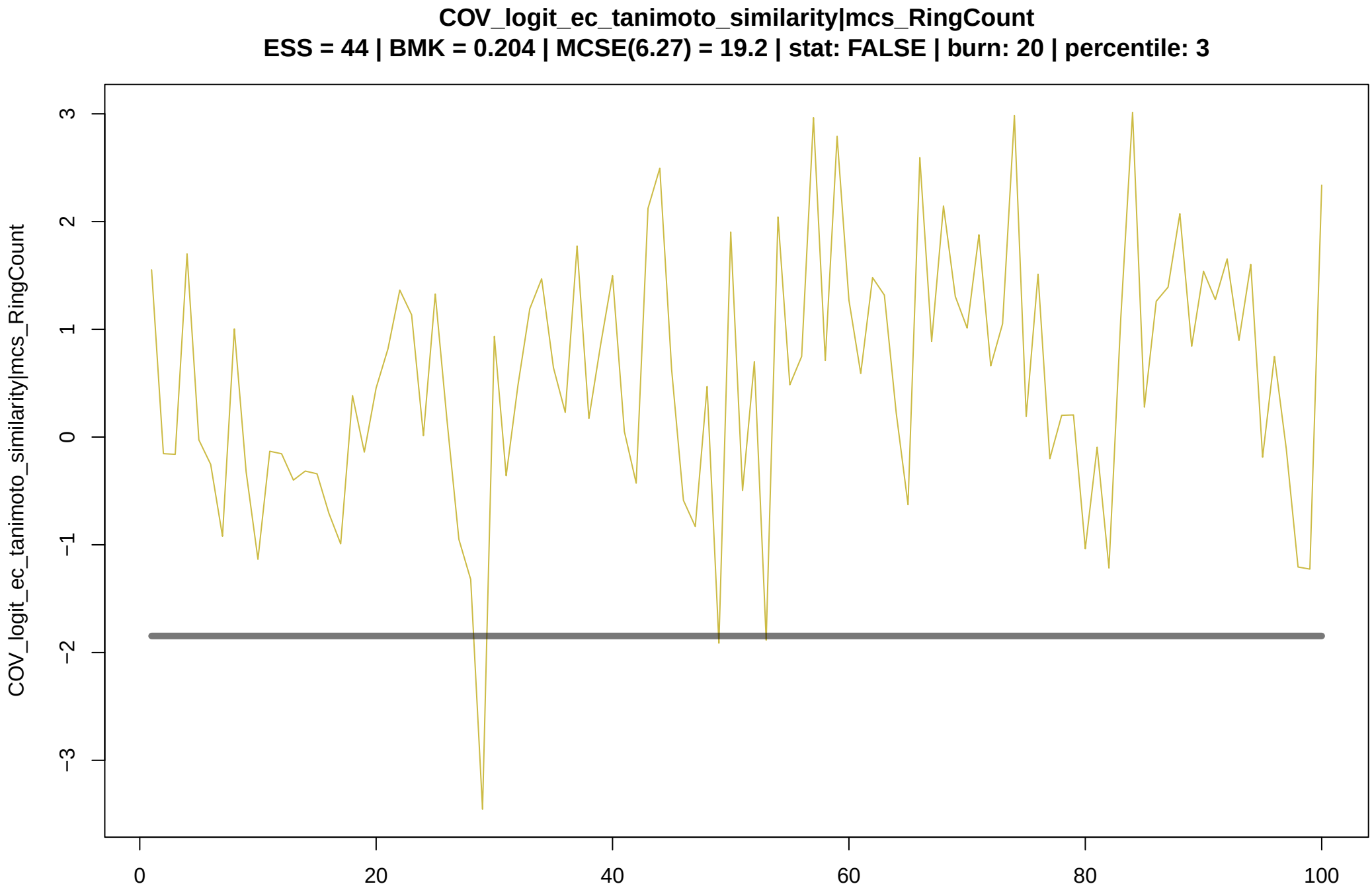

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 100 | BMK = 0.171 | MCSE(6.27) = 11.9 | stat: TRUE | burn: 0 | percentile: 26
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0
−1
−2
−3
0
20
40
60
80
100

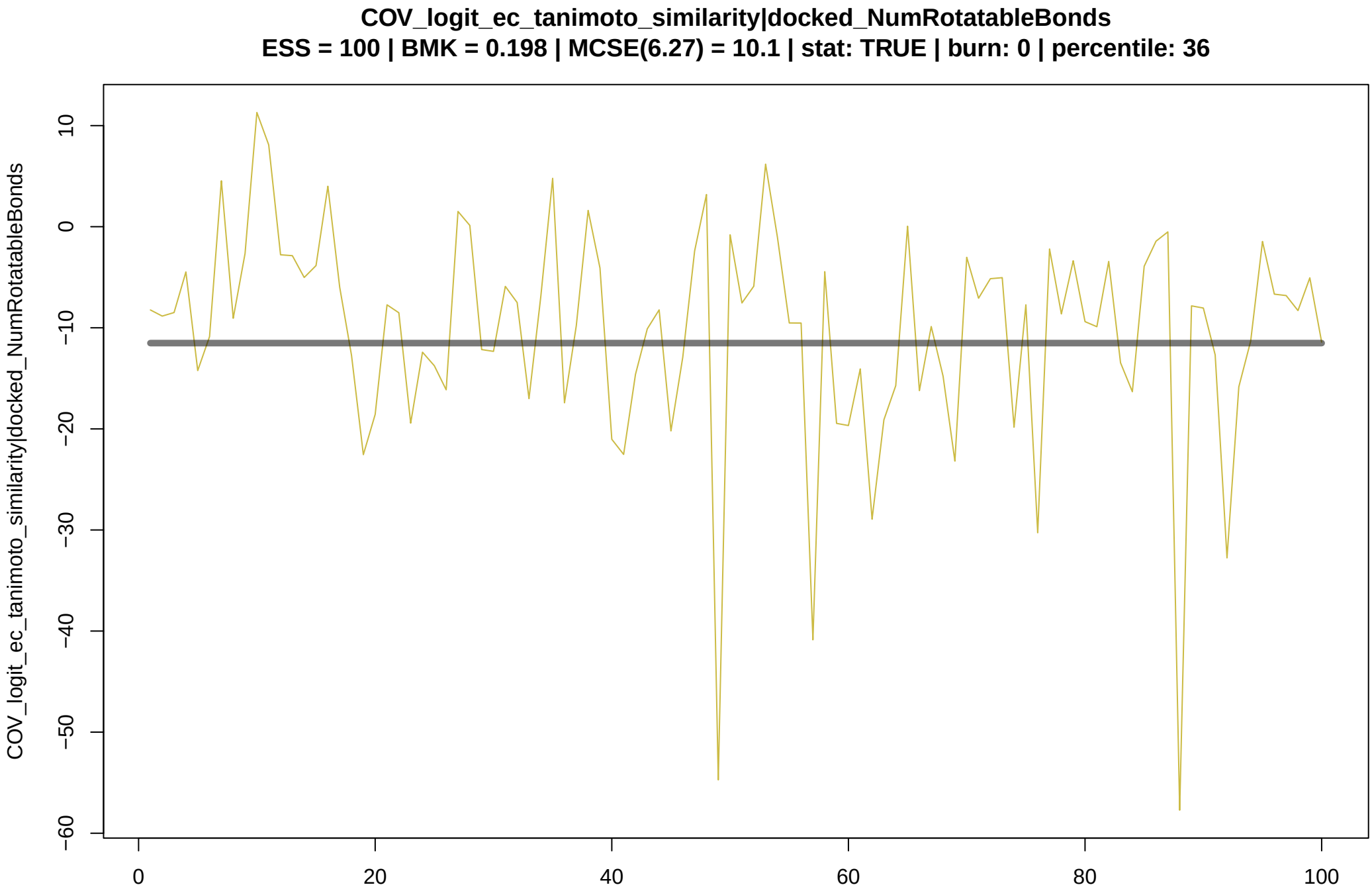

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 51.6 | BMK = 0.185 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 60 | percentile: 25
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
25
20
15
10
5
0
−5
0
20
40
60
80
100

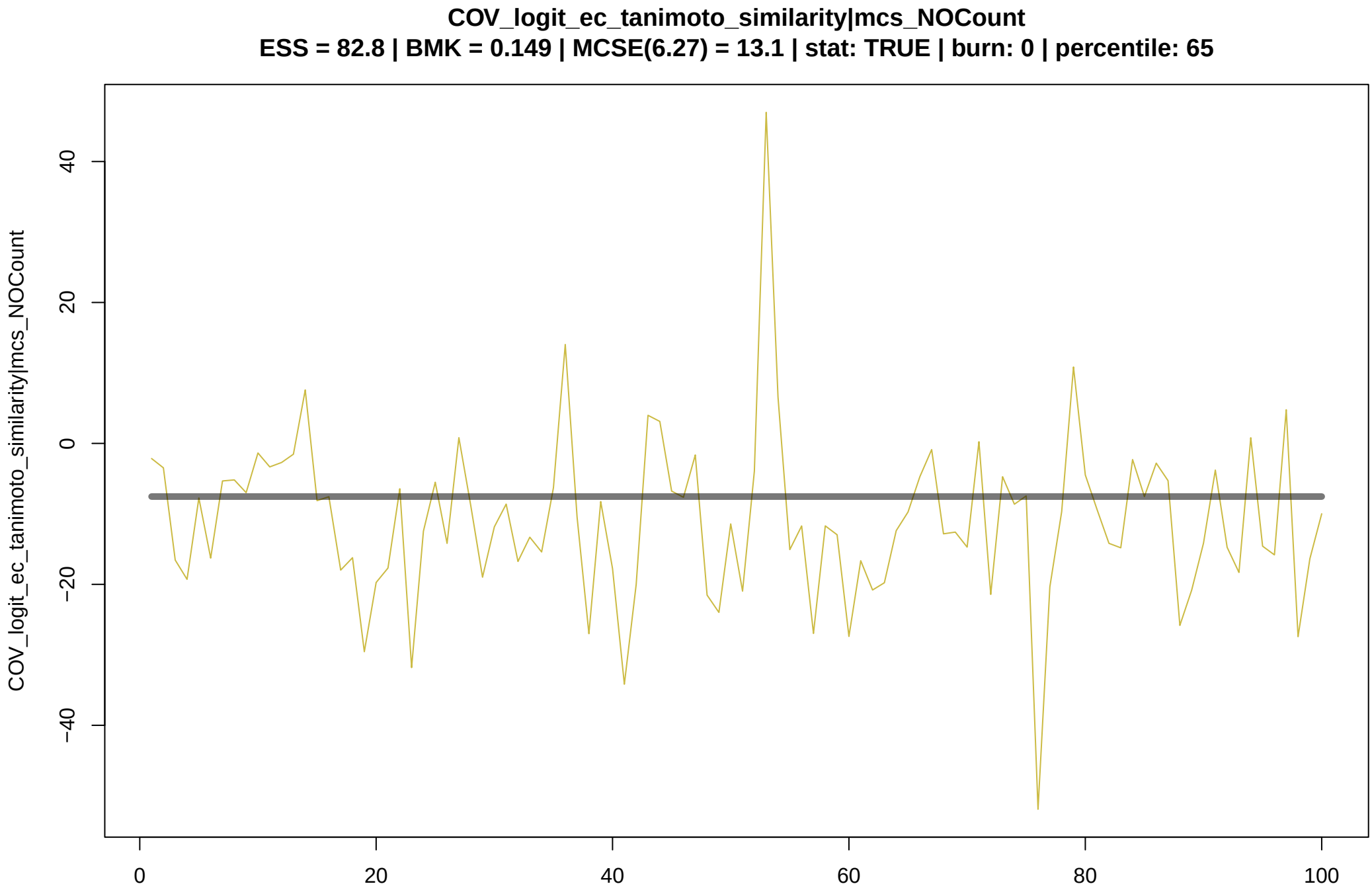

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 32.5 | BMK = 0.233 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 0 | percentile: 79
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0
−10
−20
−30
−40
0
20
40
60
80
100

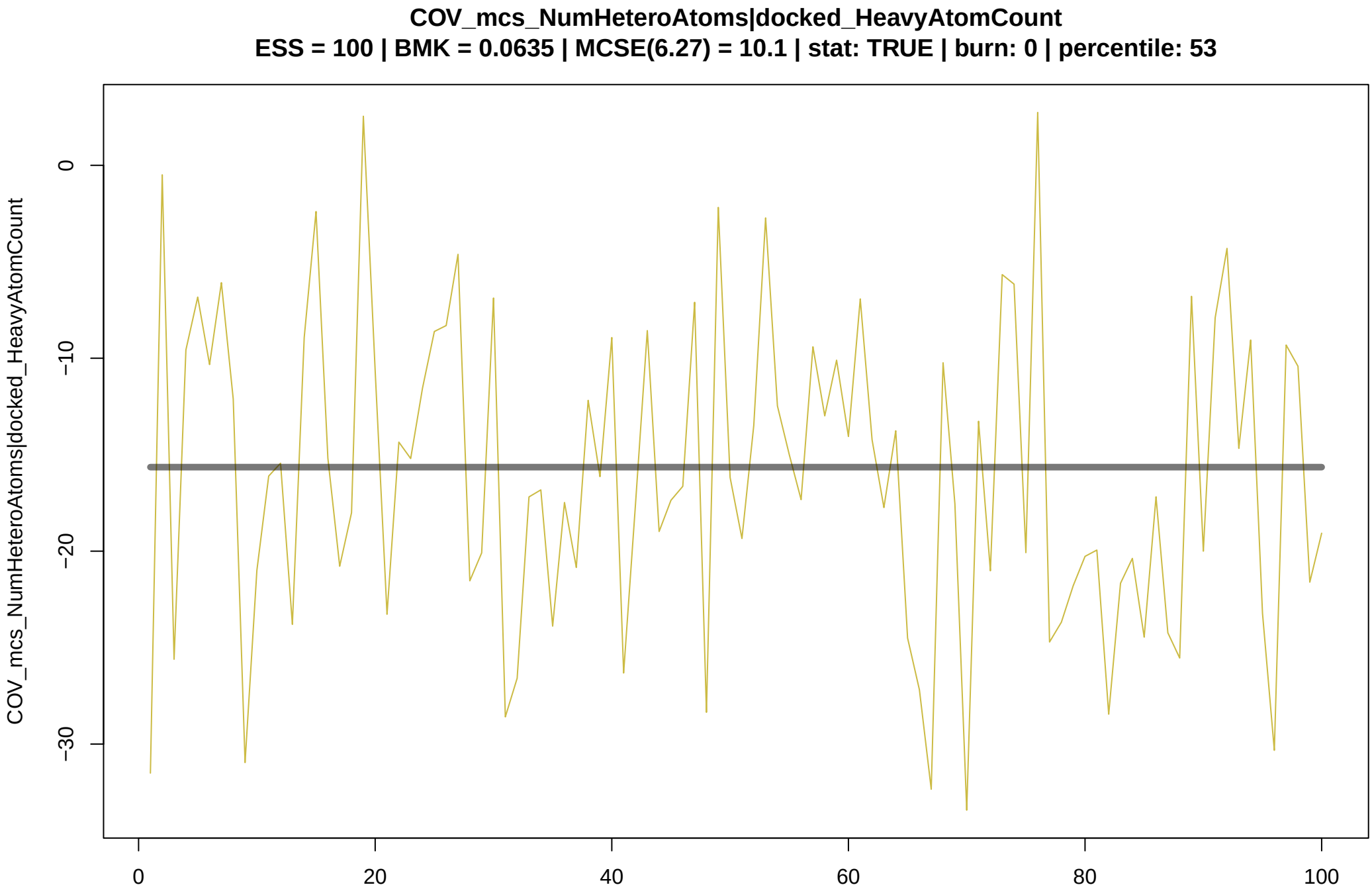

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 100 | BMK = 0.132 | MCSE(6.27) = 9.1 | stat: TRUE | burn: 100 | percentile: 34
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
2
0
−2
−4
−6
−8
0
20
40
60
80
100

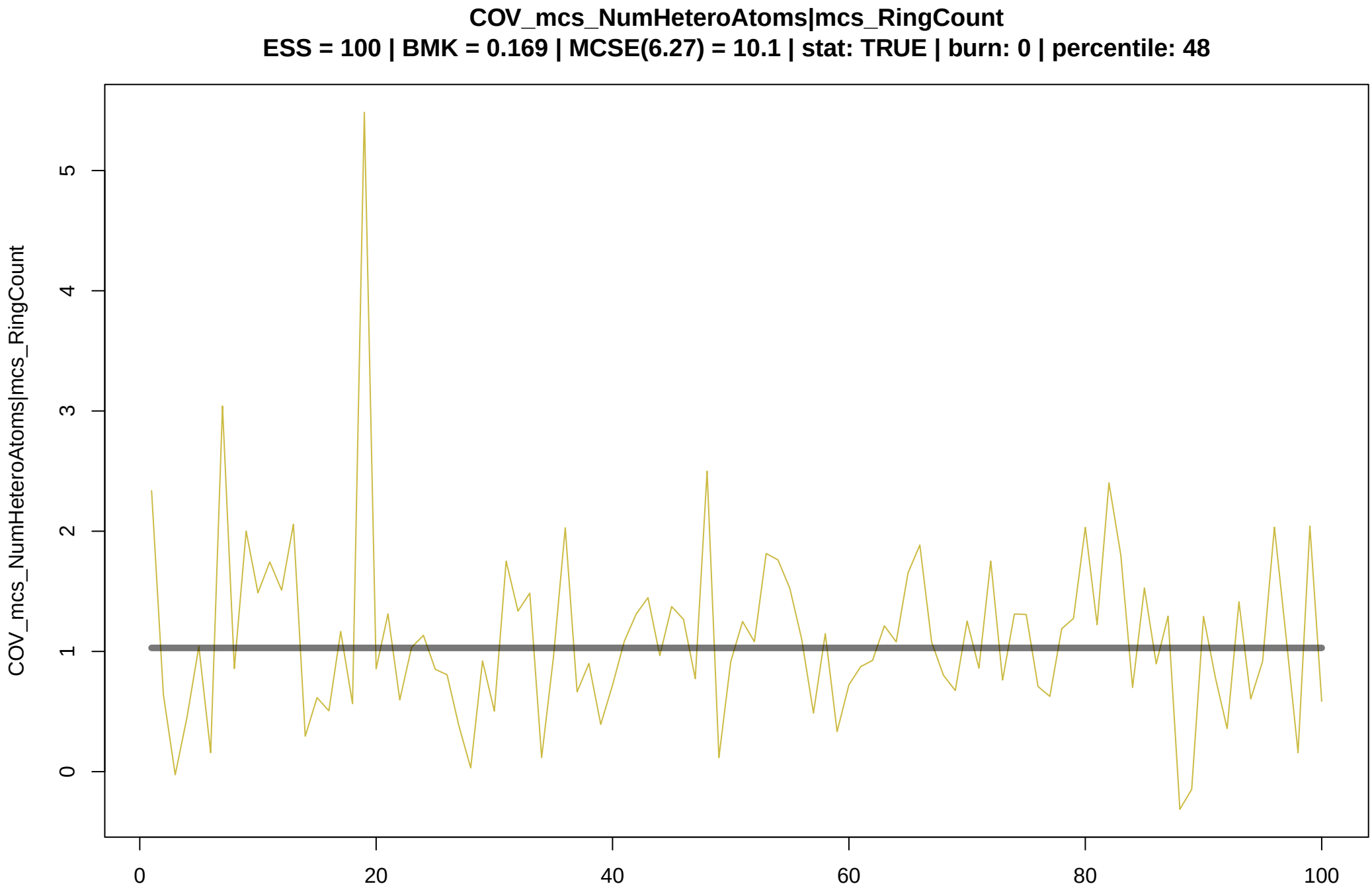

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 68.1 | BMK = 0.139 | MCSE(6.27) = 15.7 | stat: FALSE | burn: 0 | percentile: 94
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
0
10
20
30
40
50
60
0
20
40
60
80
100

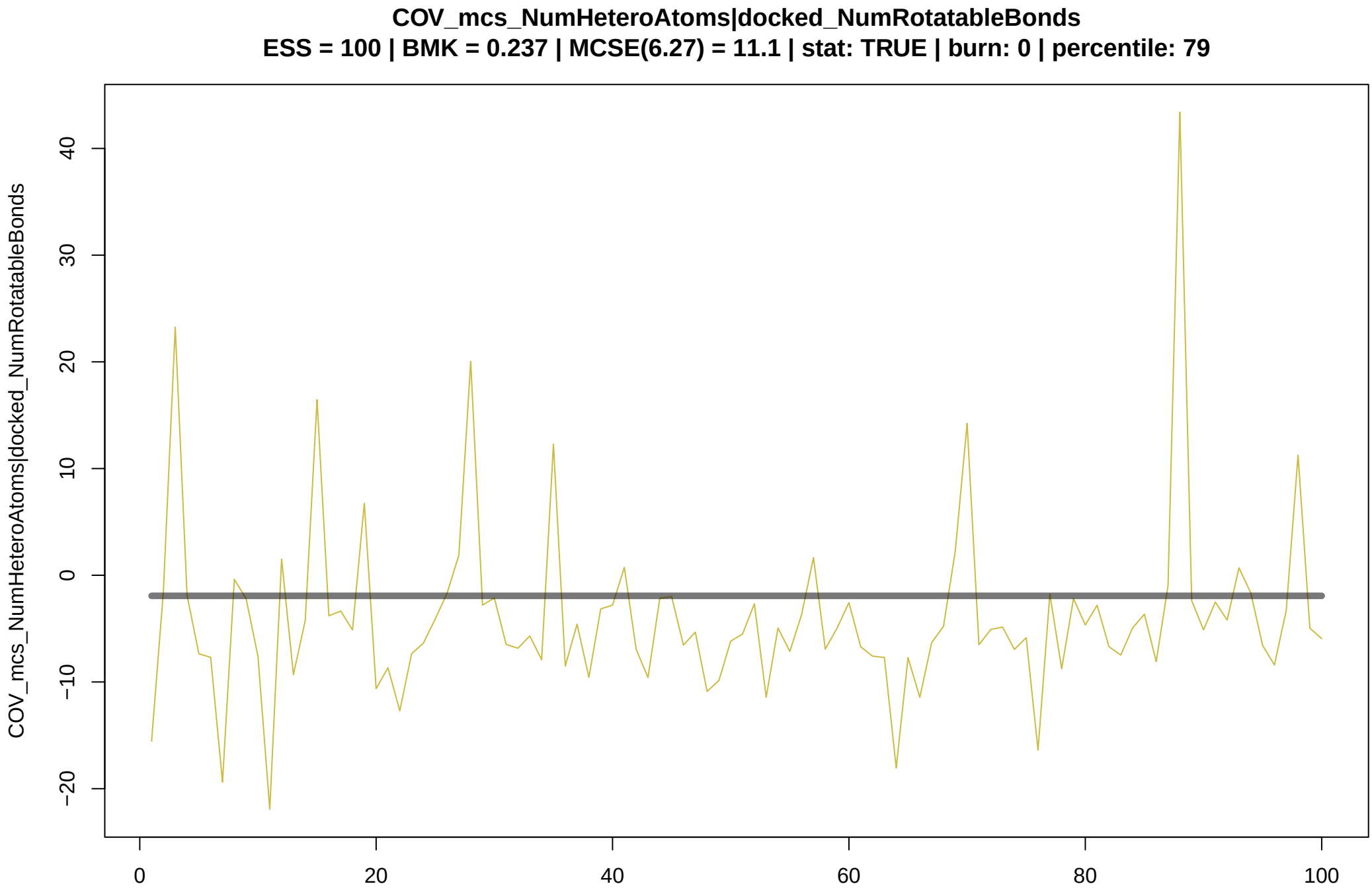

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 44 | BMK = 0.204 | MCSE(6.27) = 19.2 | stat: FALSE | burn: 20 | percentile: 3
COV_logit_ec_tanimoto_similarity|mcs_RingCount
3
2
1
0
−1
−2
−3
0
20
40
60
80
100

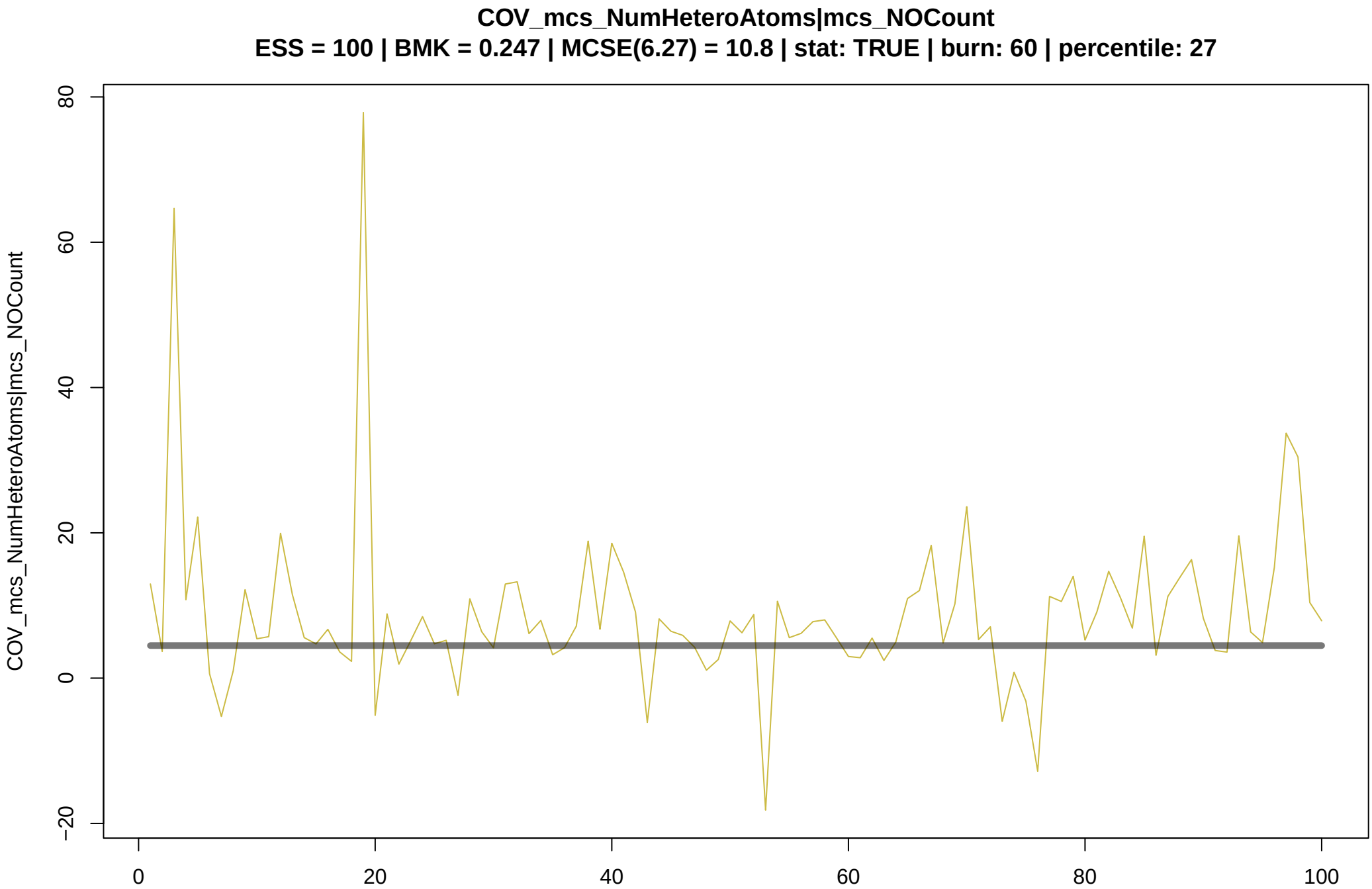

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 100 | BMK = 0.198 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0 | percentile: 36
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
10
0
−10
−20
−30
−40
−50
−60
0
20
40
60
80
100

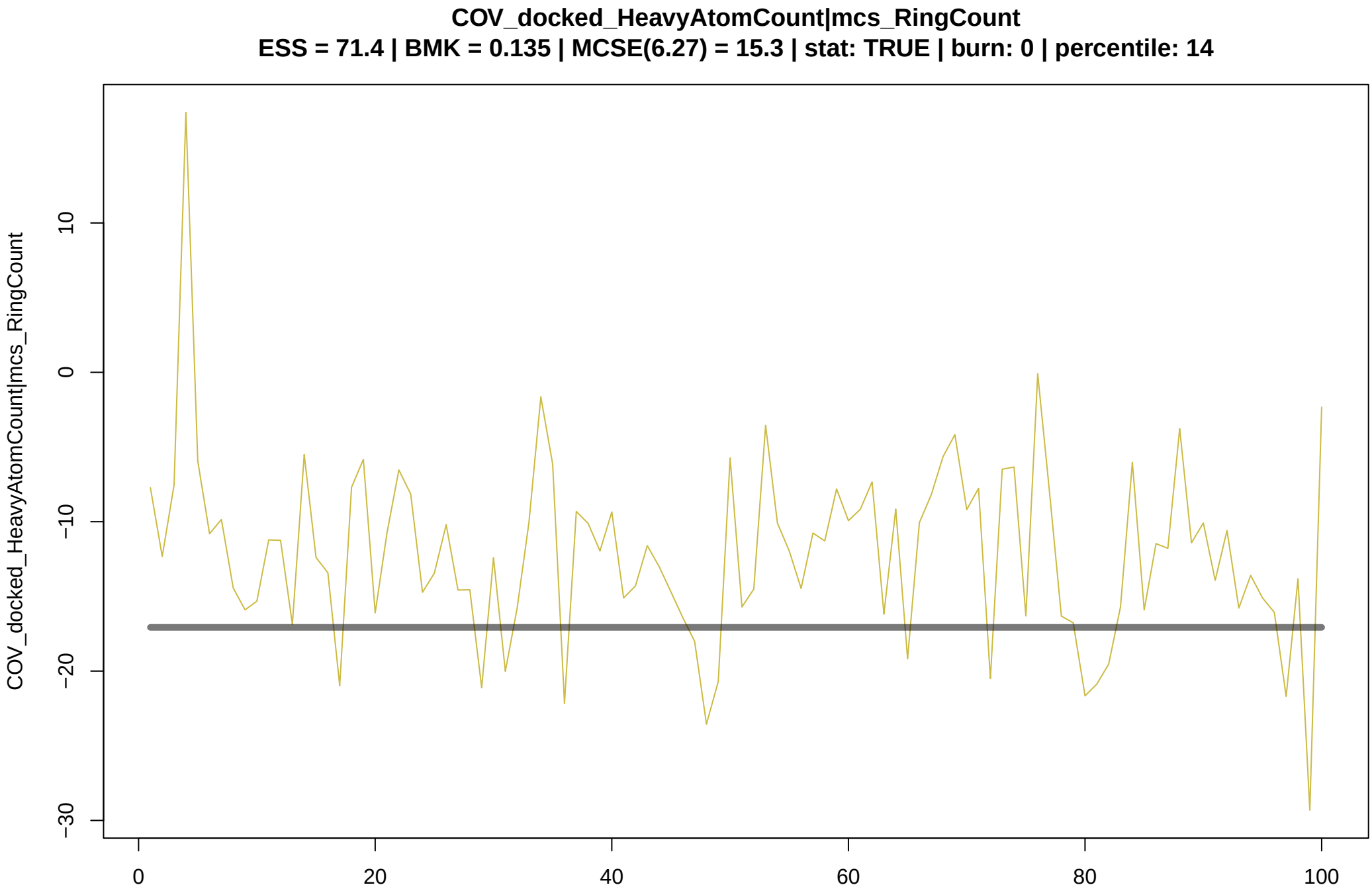

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 82.8 | BMK = 0.149 | MCSE(6.27) = 13.1 | stat: TRUE | burn: 0 | percentile: 65
COV_logit_ec_tanimoto_similarity|mcs_NOCount
40
20
0
−20
−40
0
20
40
60
80
100

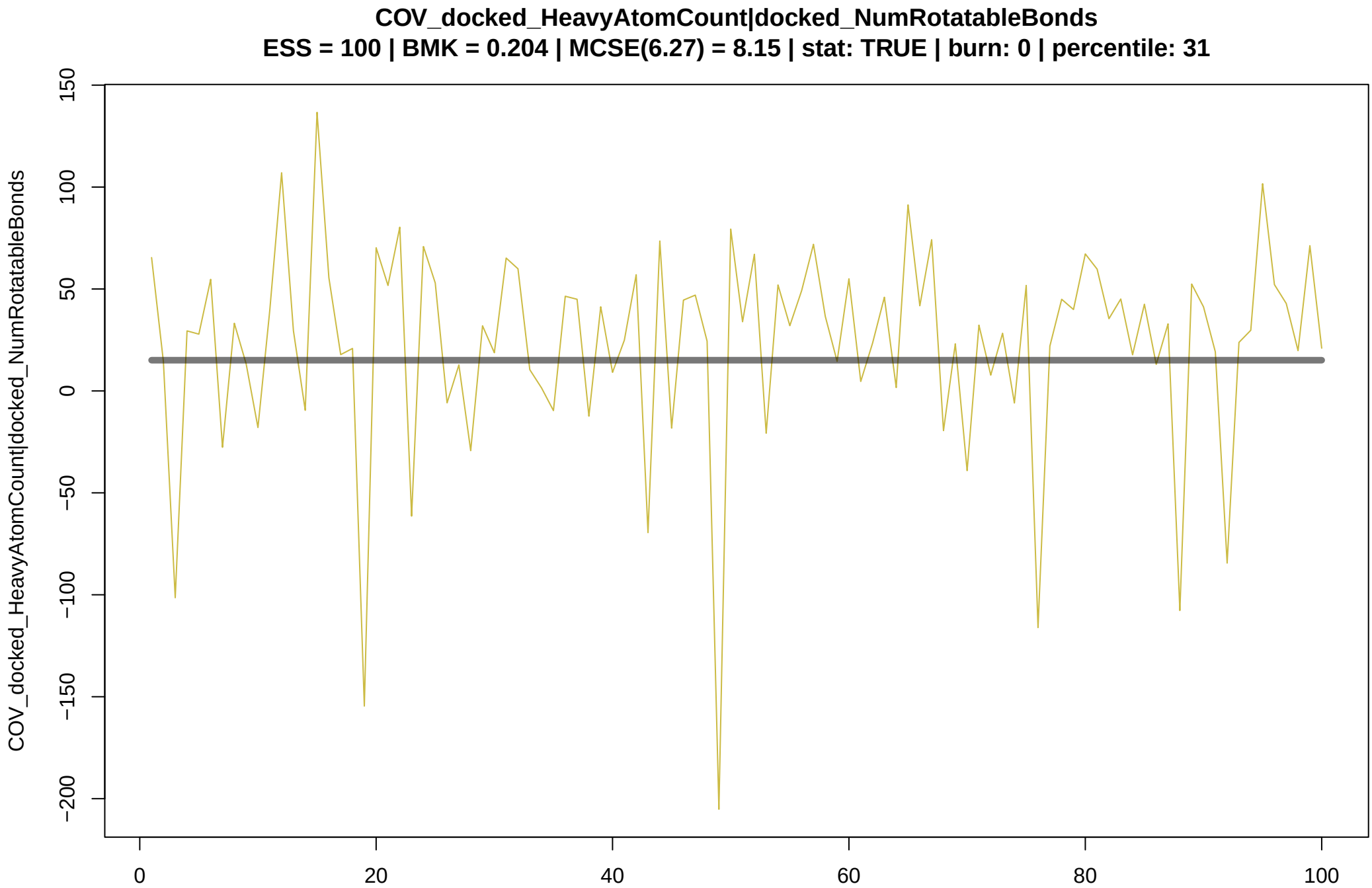

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 100 | BMK = 0.0635 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0 | percentile: 53
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
0
−10
−20
−30
0
20
40
60
80
100

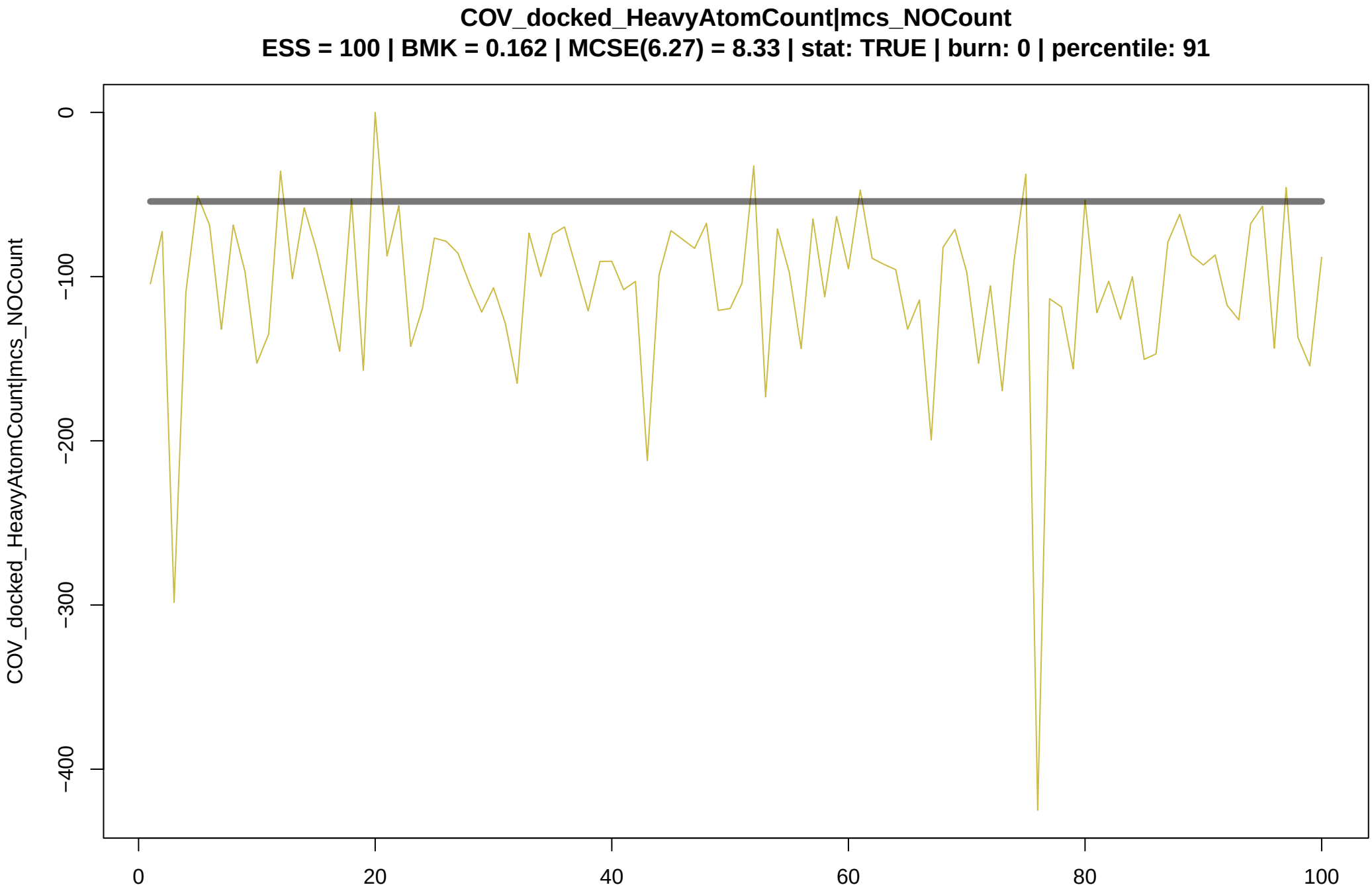

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 100 | BMK = 0.169 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0 | percentile: 48
COV_mcs_NumHeteroAtoms|mcs_RingCount
0
1
2
3
4
5
0
20
40
60
80
100

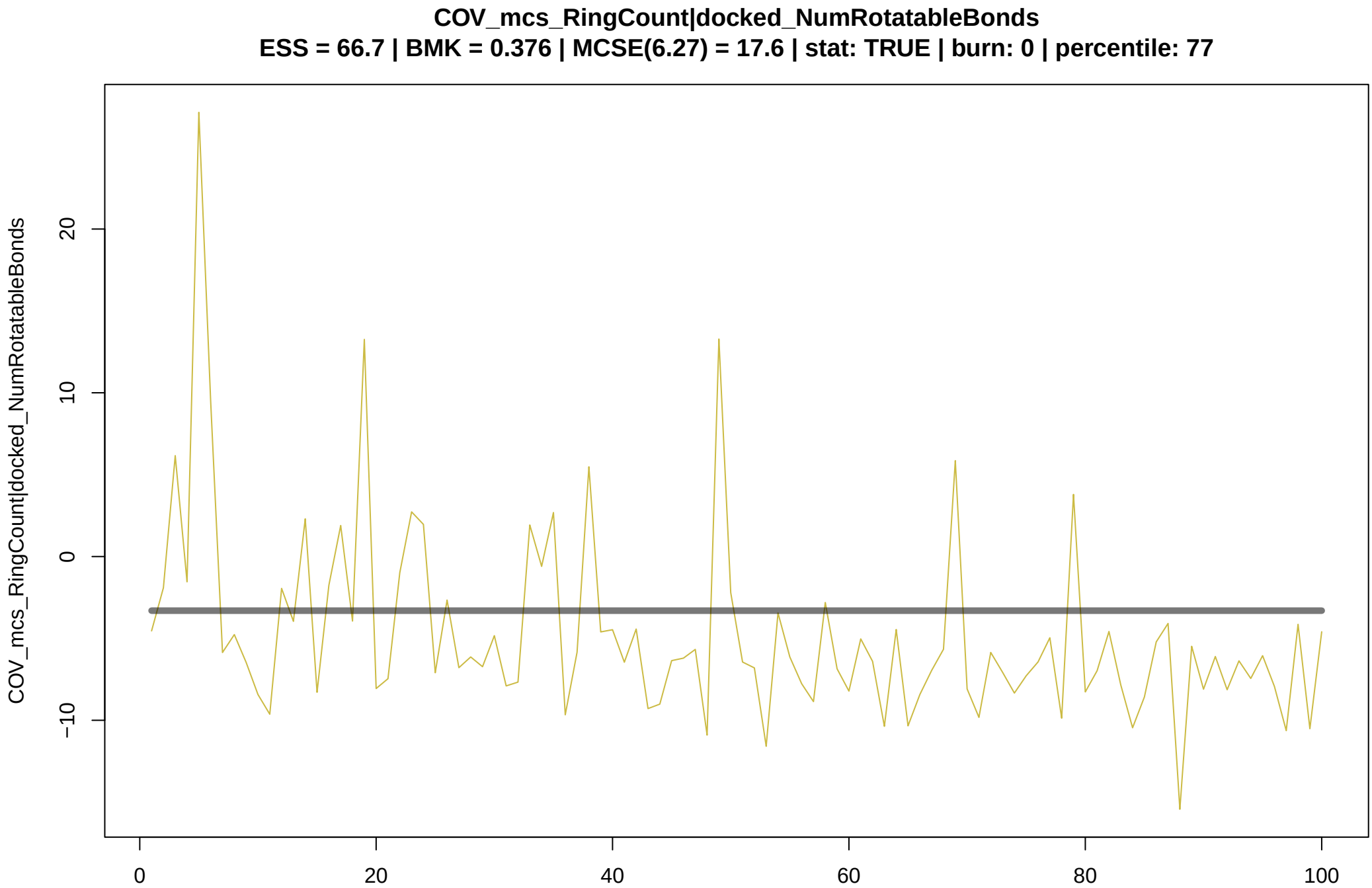

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 100 | BMK = 0.237 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0 | percentile: 79
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
40
30
20
10
0
−10
−20
0
20
40
60
80
100

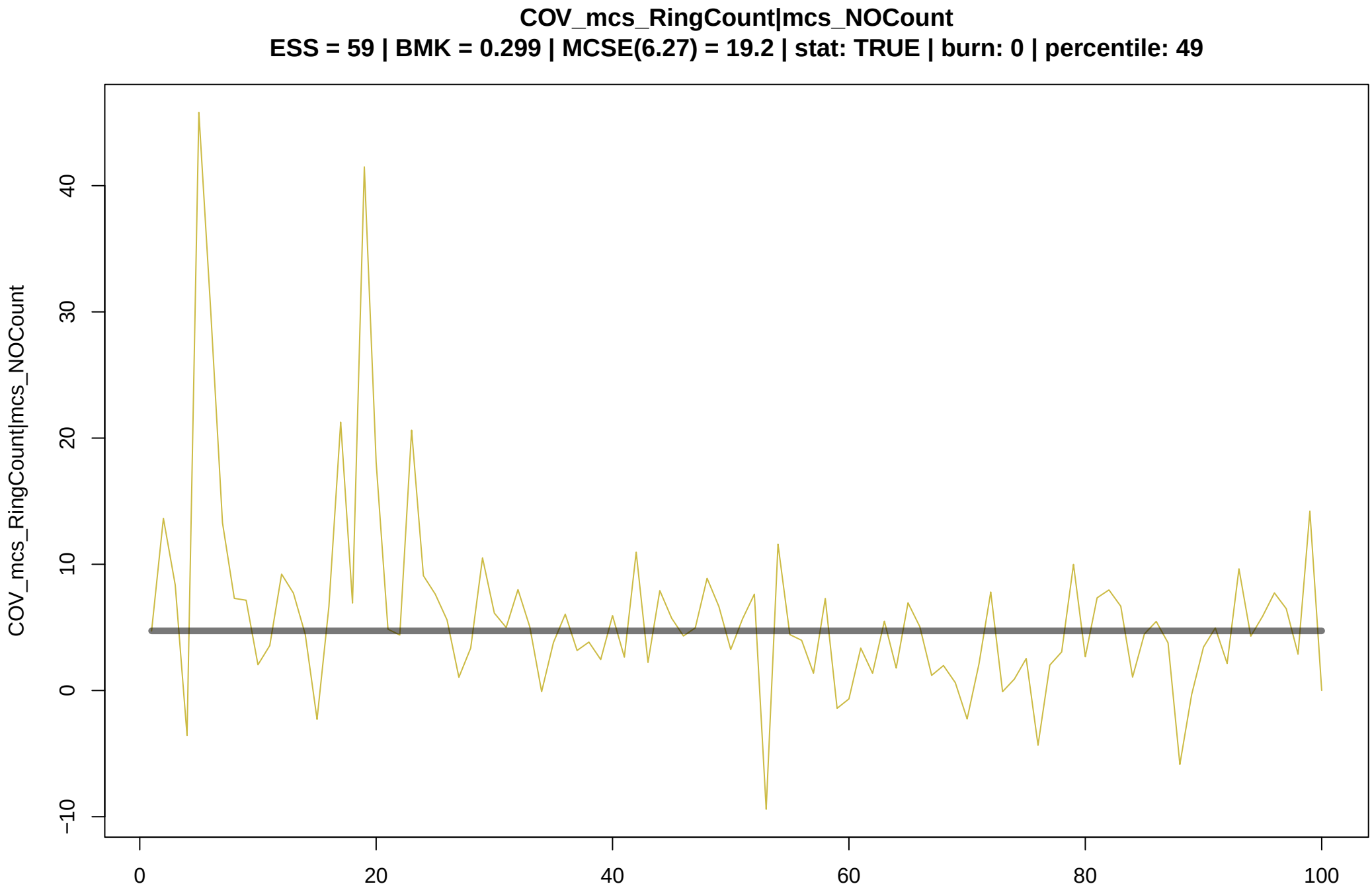

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 100 | BMK = 0.247 | MCSE(6.27) = 10.8 | stat: TRUE | burn: 60 | percentile: 27
COV_mcs_NumHeteroAtoms|mcs_NOCount
80
60
40
20
0
−20
0
20
40
60
80
100

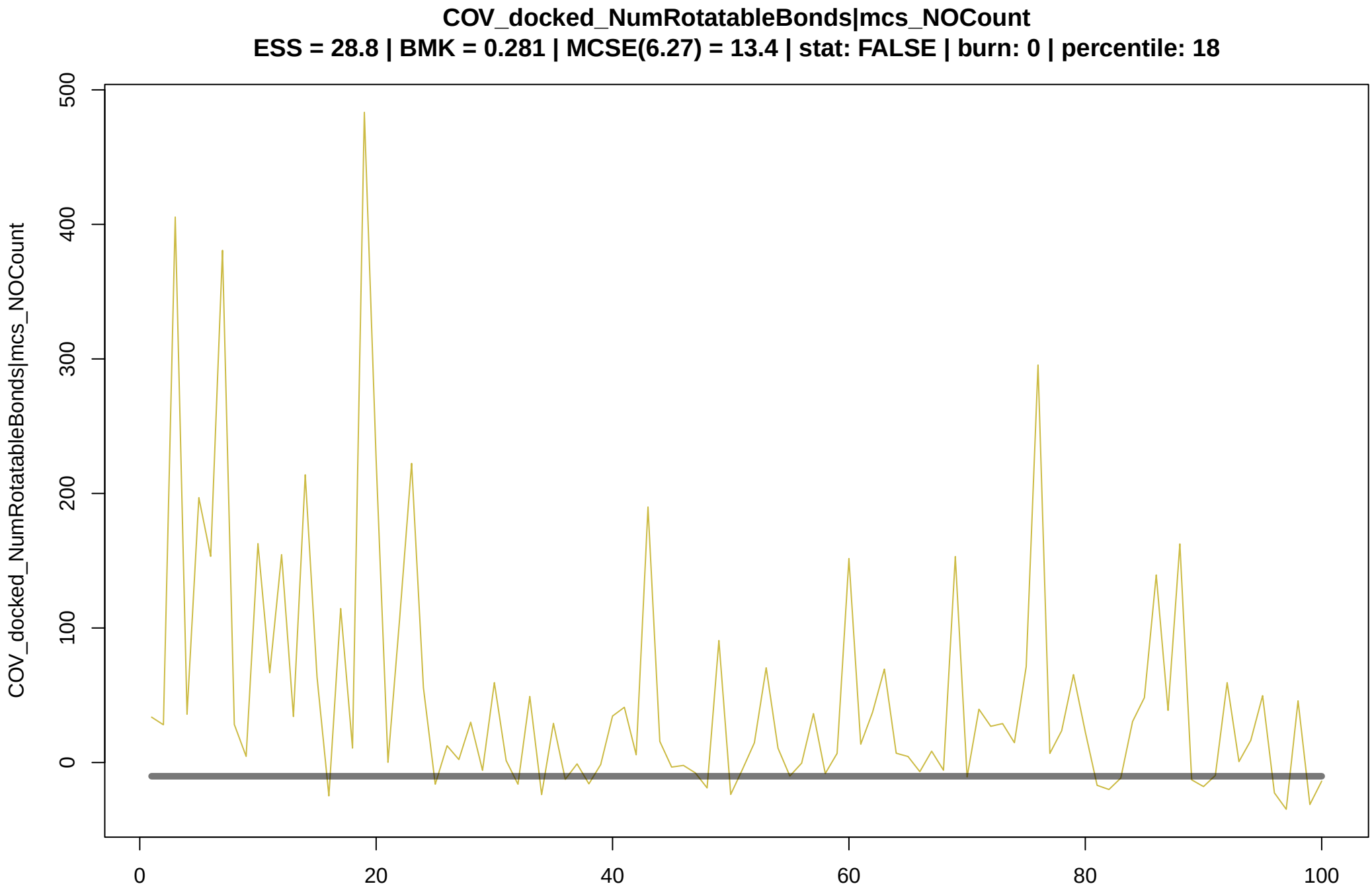

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 71.4 | BMK = 0.135 | MCSE(6.27) = 15.3 | stat: TRUE | burn: 0 | percentile: 14
COV_docked_HeavyAtomCount|mcs_RingCount
10
0
−10
−20
−30
0
20
40
60
80
100


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 100 | BMK = 0.204 | MCSE(6.27) = 8.15 | stat: TRUE | burn: 0 | percentile: 31
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
150
100
50
0
−50
−100
−150
−200
0
20
40
60
80
100


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 100 | BMK = 0.162 | MCSE(6.27) = 8.33 | stat: TRUE | burn: 0 | percentile: 91
COV_docked_HeavyAtomCount|mcs_NOCount
0
−100
−200
−300
−400
0
20
40
60
80
100


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 66.7 | BMK = 0.376 | MCSE(6.27) = 17.6 | stat: TRUE | burn: 0 | percentile: 77
COV_mcs_RingCount|docked_NumRotatableBonds
20
10
0
−10
0
20
40
60
80
100


COV_mcs_RingCount|mcs_NOCount
ESS = 59 | BMK = 0.299 | MCSE(6.27) = 19.2 | stat: TRUE | burn: 0 | percentile: 49
COV_mcs_RingCount|mcs_NOCount
−10
0
10
20
30
40
0
20
40
60
80
100


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 28.8 | BMK = 0.281 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0 | percentile: 18
COV_docked_NumRotatableBonds|mcs_NOCount
0
100
200
300
400
500
0
20
40
60
80
100