-- STATS maxD --

min ESS = 176.898720586097

max BMK = 0.121776434400169

max MCSE = 6.16587908344426

all stationary: FALSE

burn: 0

max rel.err.: 2.06318844924603

-- STATS 1D --

min ESS = 2031.42633598623

max BMK = 0.0522965032716056

max MCSE = 2.50647748295101

all stationary: FALSE

burn: 0

max rel.err.: 2.26804424466483

-- STATS 2D --

min ESS = 3379.87273503769

max BMK = 0.040659346825983

max MCSE = 1.96506149114878

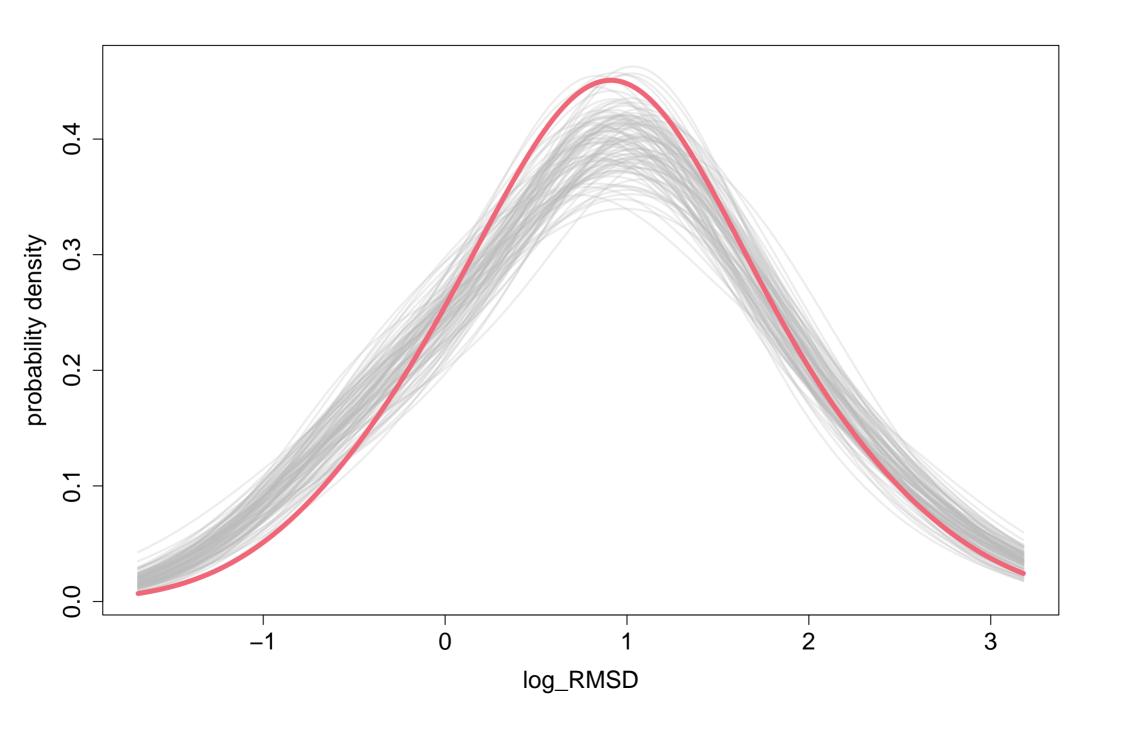
all stationary: FALSE

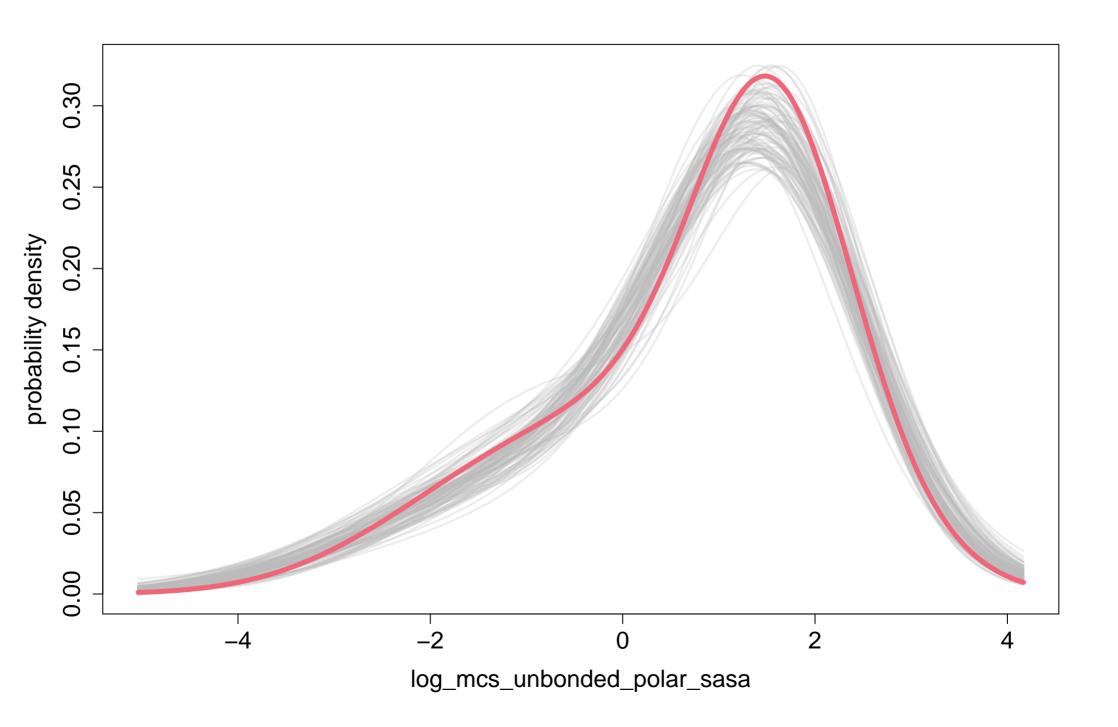
burn: 0

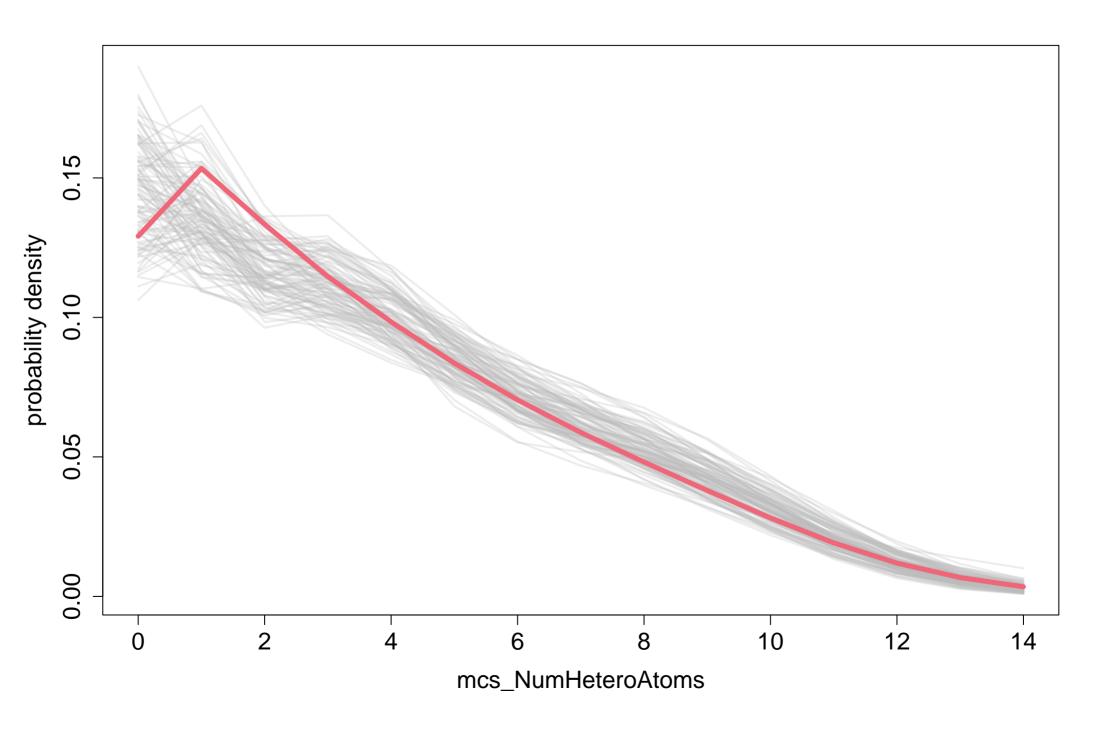
max rel.err.: 1.7621698578807

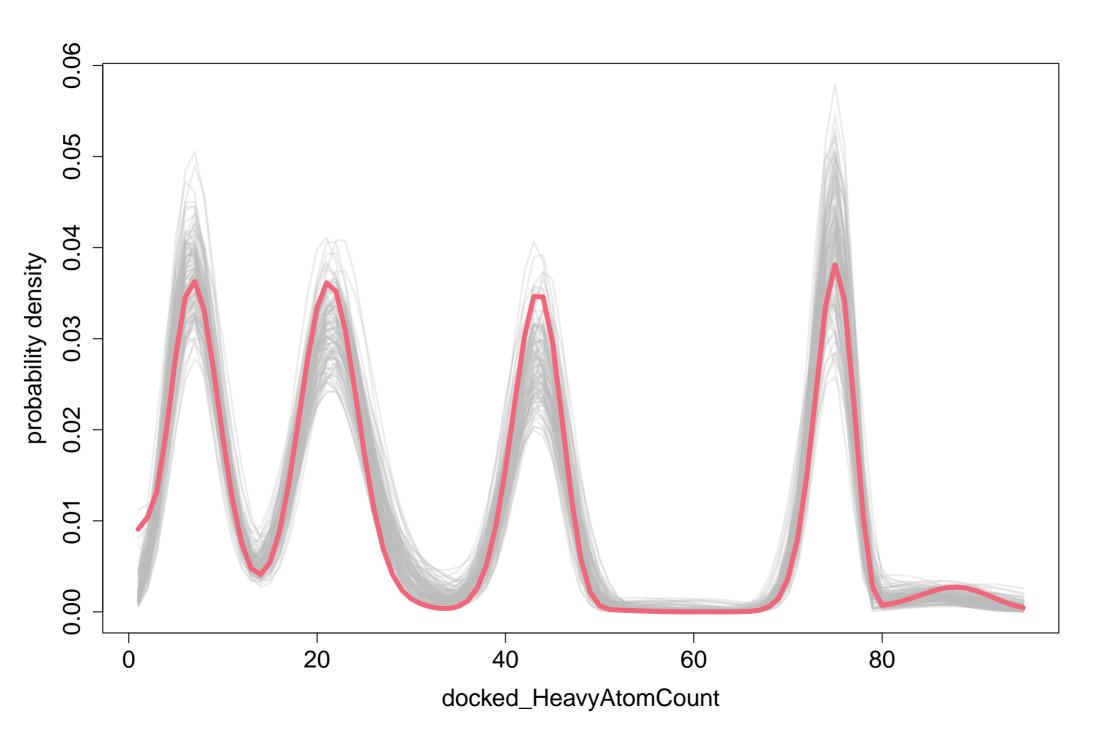
Occupied clusters: 9 of 16

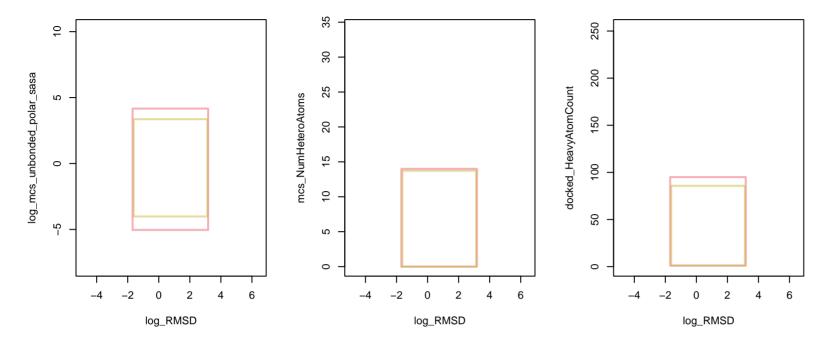
LL: -2160 +- 6.63

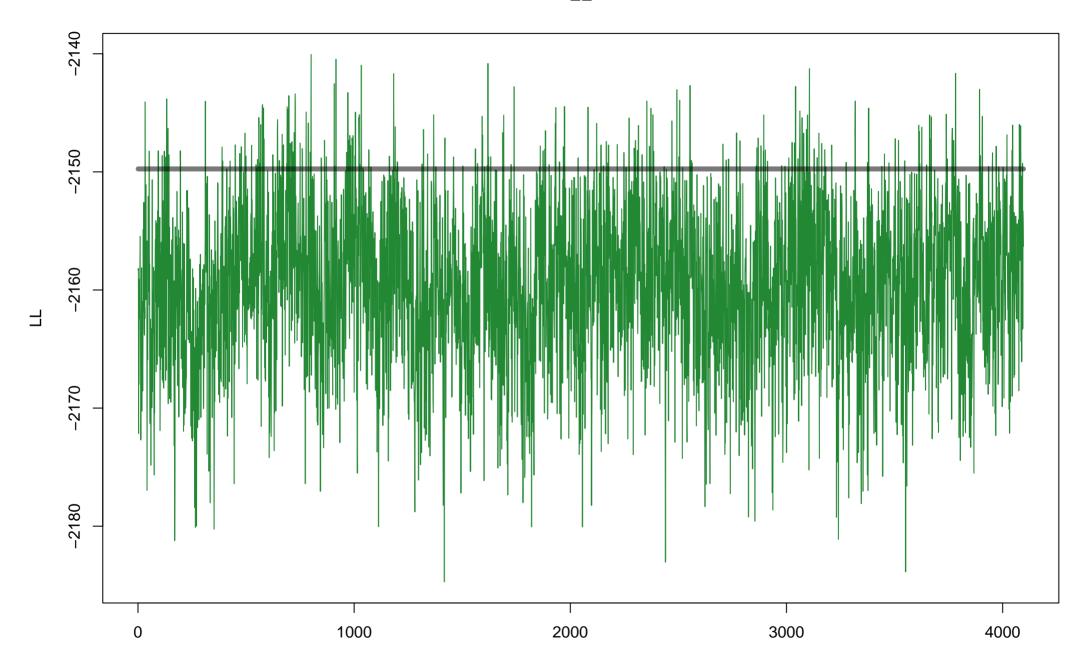






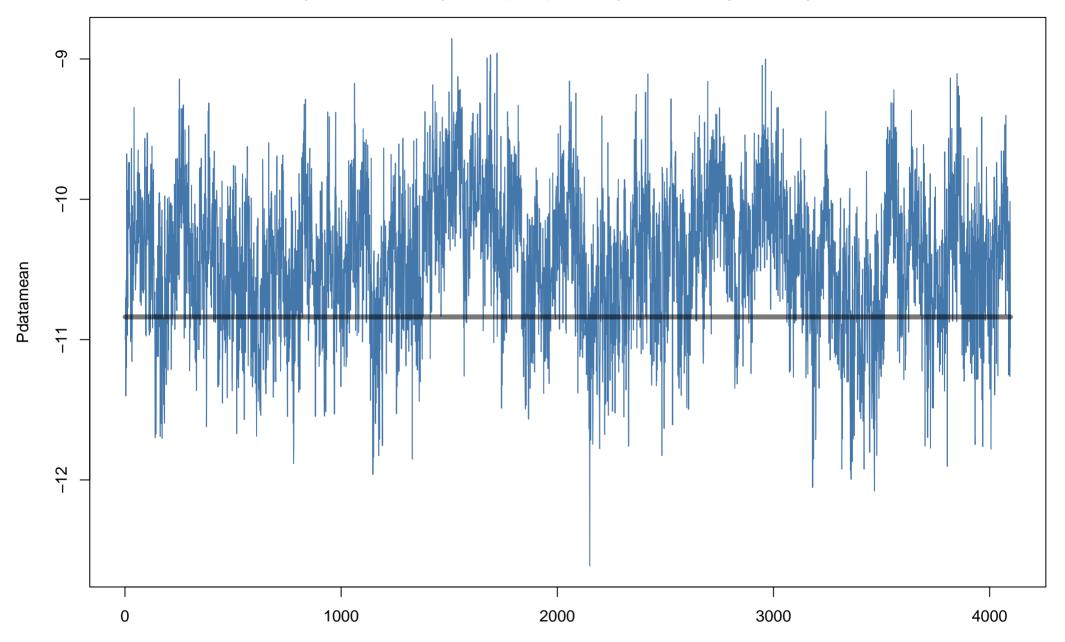




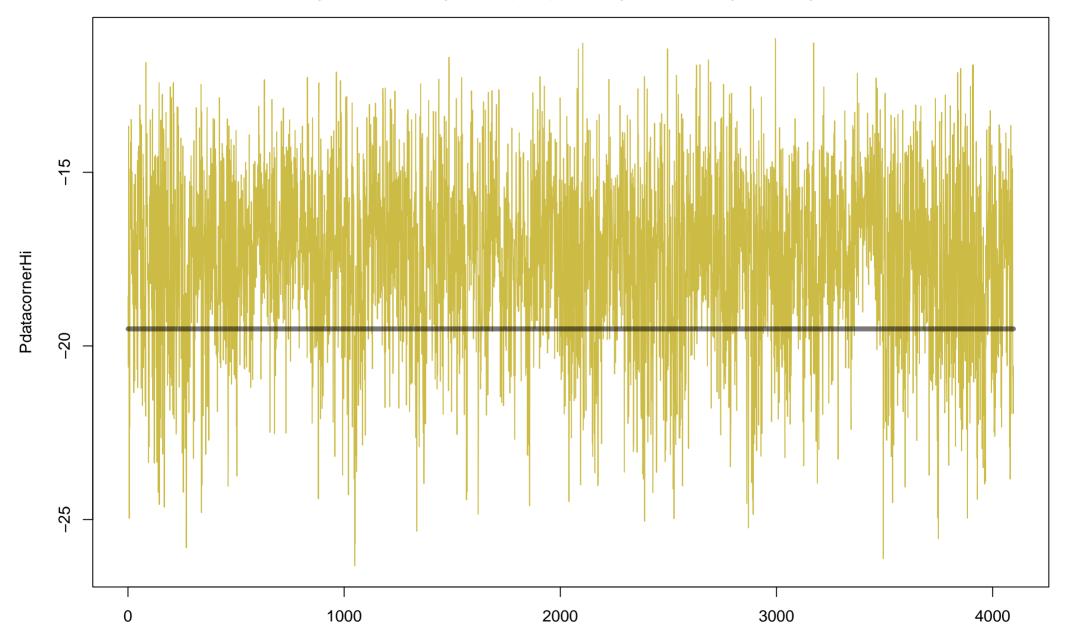


Pdatamean

ESS = 177 | BMK = 0.0413 | MCSE(6.27) = 6.17 | stat: TRUE | burn: 0 | rel.err: 0.821

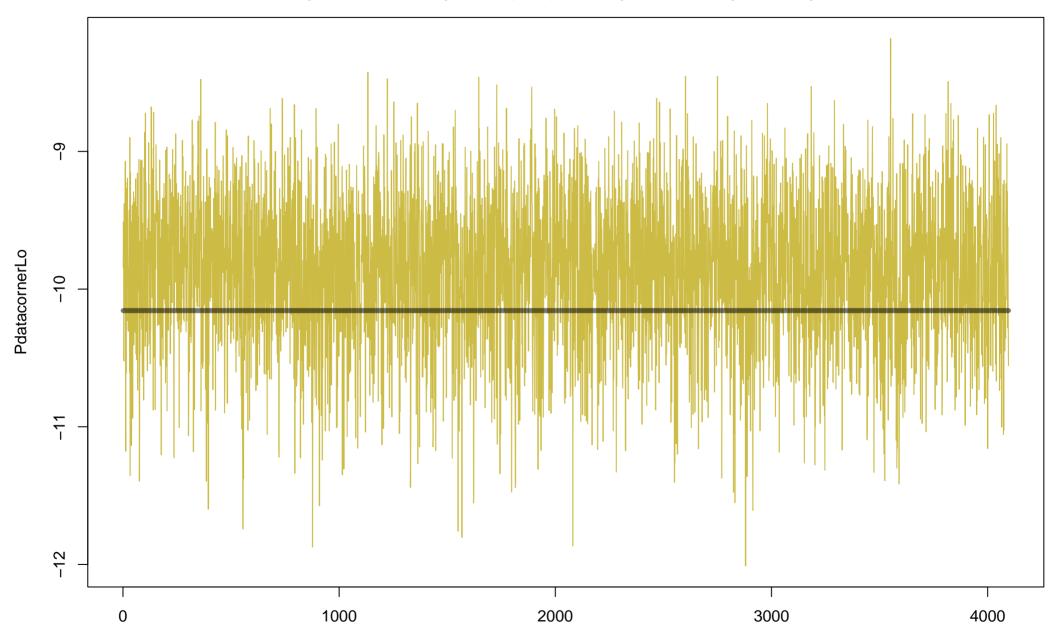


PdatacornerHi
ESS = 4100 | BMK = 0.122 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: 0.301



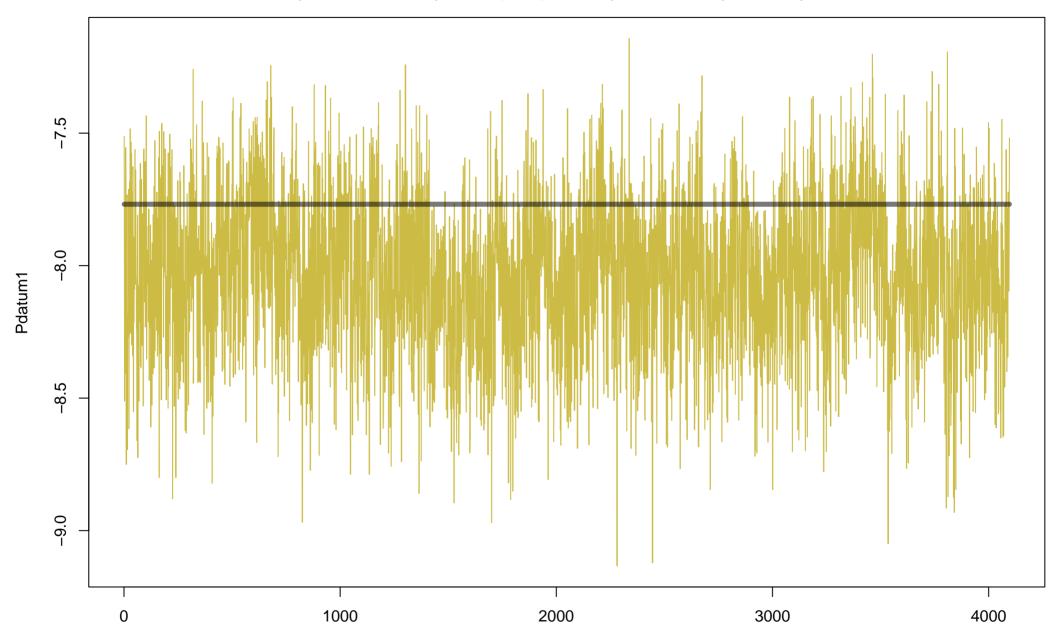
PdatacornerLo

ESS = 3540 | BMK = 0.0334 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 0.668

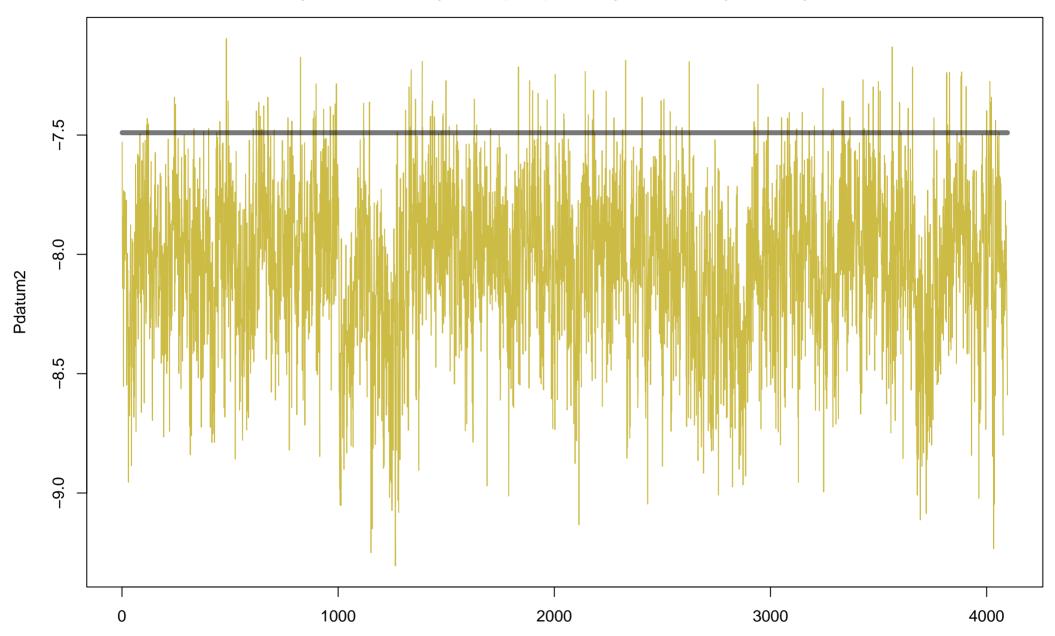


Pdatum1

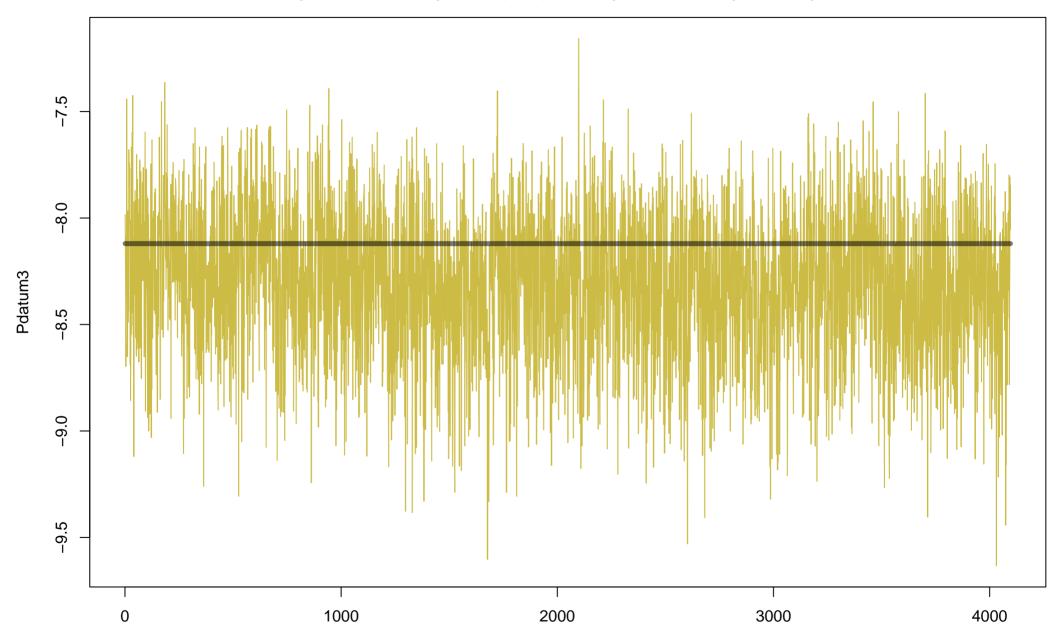
ESS = 768 | BMK = 0.0338 | MCSE(6.27) = 3.82 | stat: TRUE | burn: 0 | rel.err: -0.889



Pdatum2 ESS = 388 | BMK = 0.0485 | MCSE(6.27) = 4.57 | stat: TRUE | burn: 0 | rel.err: -2.06

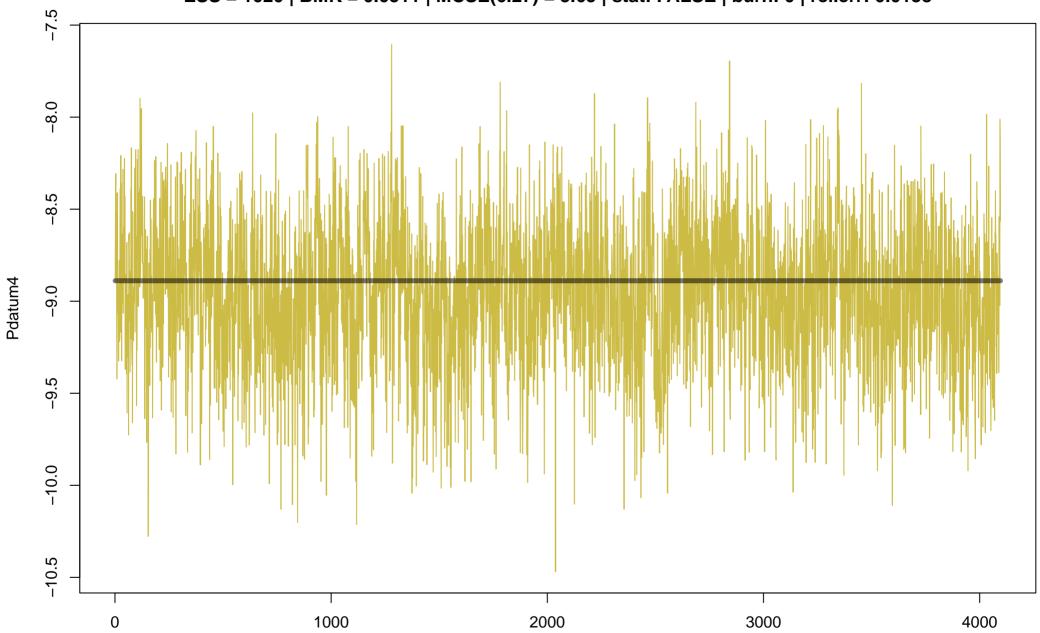


Pdatum3 ESS = 1190 | BMK = 0.0551 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0 | rel.err: -0.403



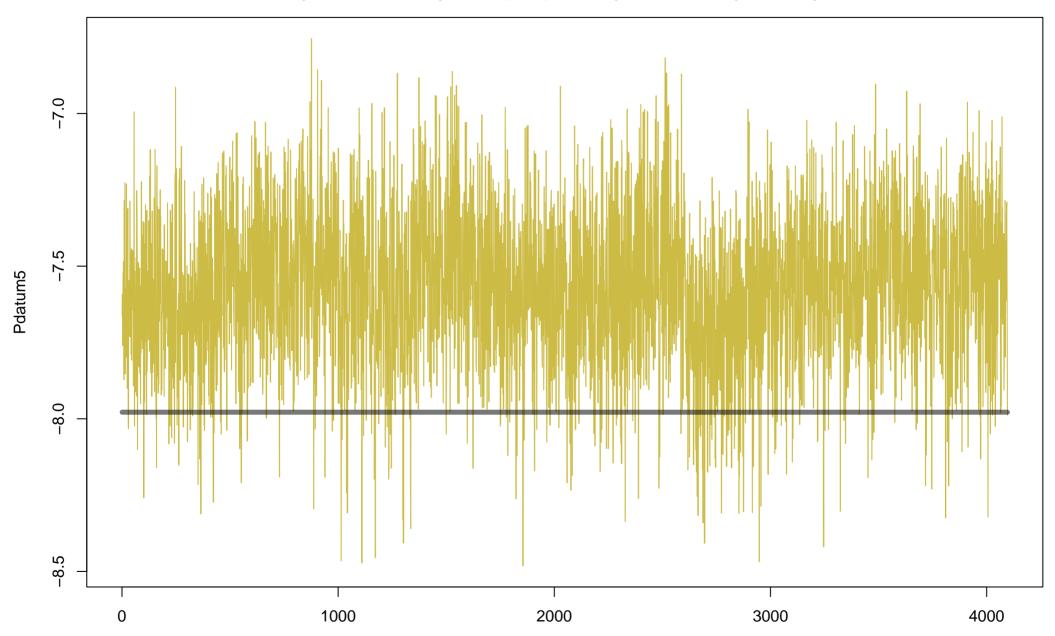
Pdatum4

ESS = 1020 | BMK = 0.0511 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0 | rel.err: 0.0138



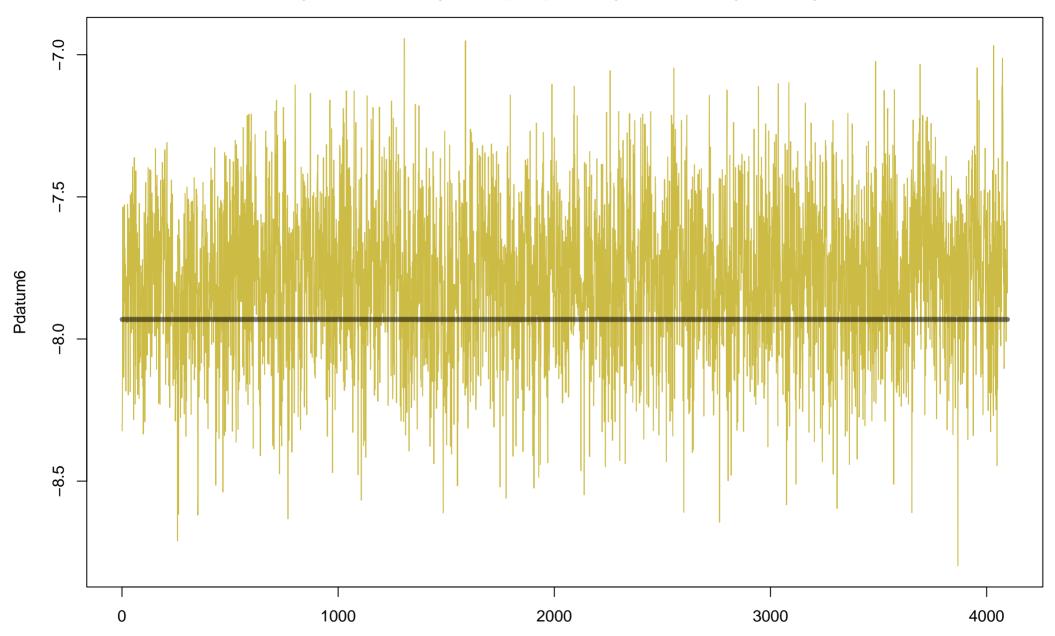
Pdatum5

ESS = 502 | BMK = 0.0412 | MCSE(6.27) = 3.39 | stat: FALSE | burn: 0 | rel.err: 1.41



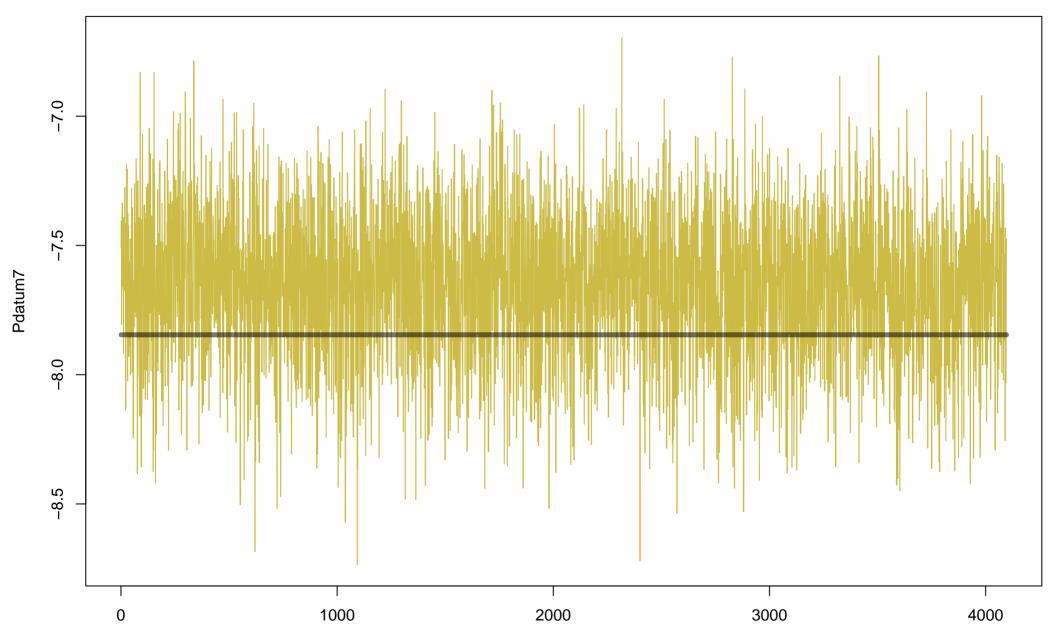
Pdatum6

ESS = 1940 | BMK = 0.0433 | MCSE(6.27) = 2.49 | stat: FALSE | burn: 0 | rel.err: 0.616

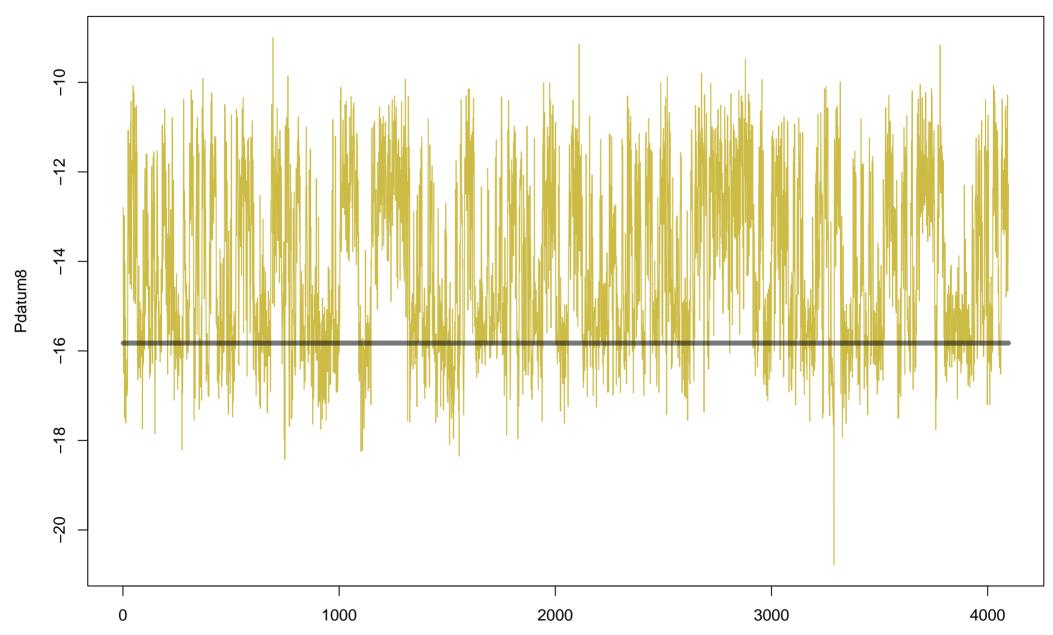


Pdatum7

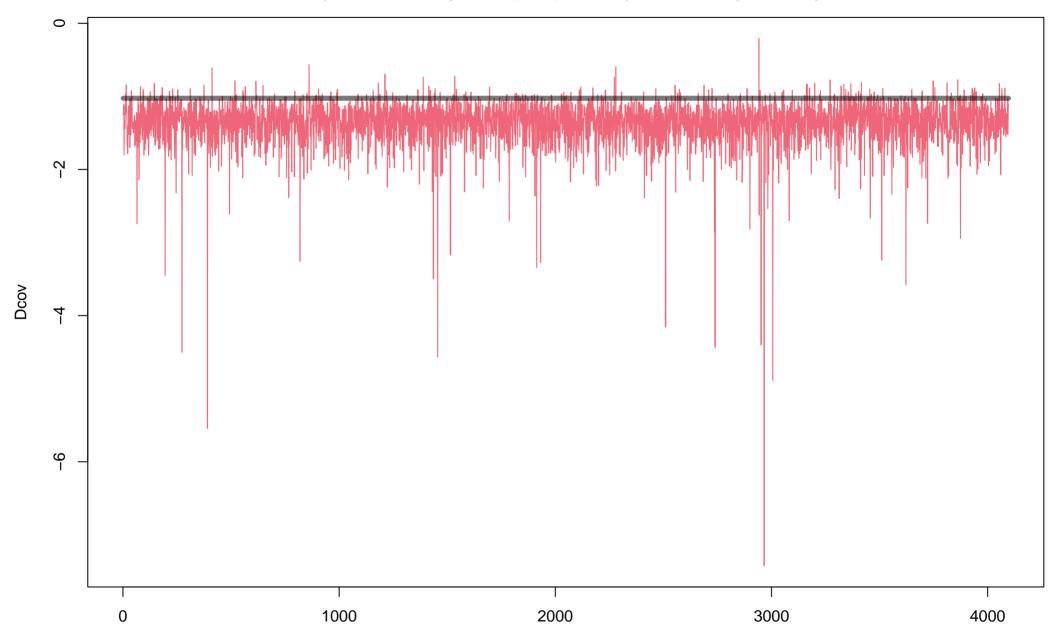
ESS = 3410 | BMK = 0.0398 | MCSE(6.27) = 1.69 | stat: FALSE | burn: 0 | rel.err: 0.736



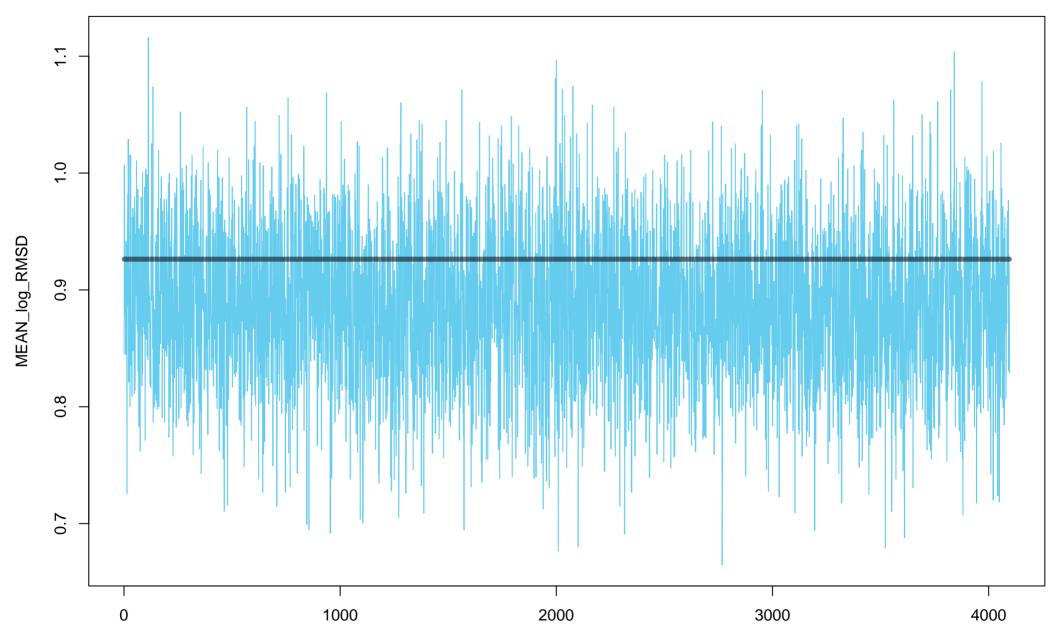
Pdatum8 ESS = 441 | BMK = 0.0861 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: 0.487



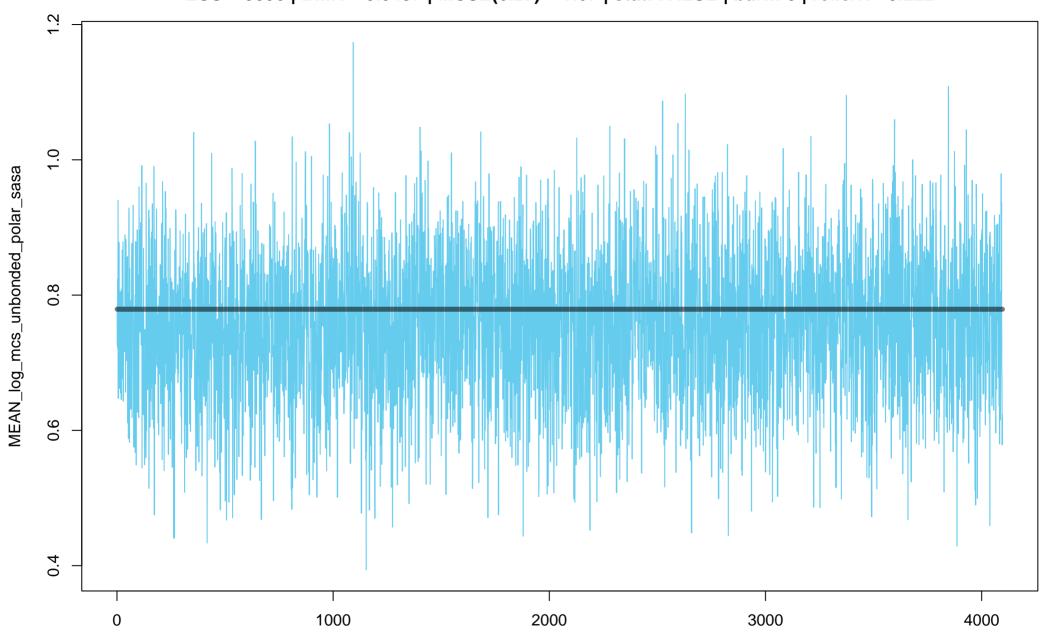
Dcov ESS = 3740 | BMK = 0.055 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 1.4



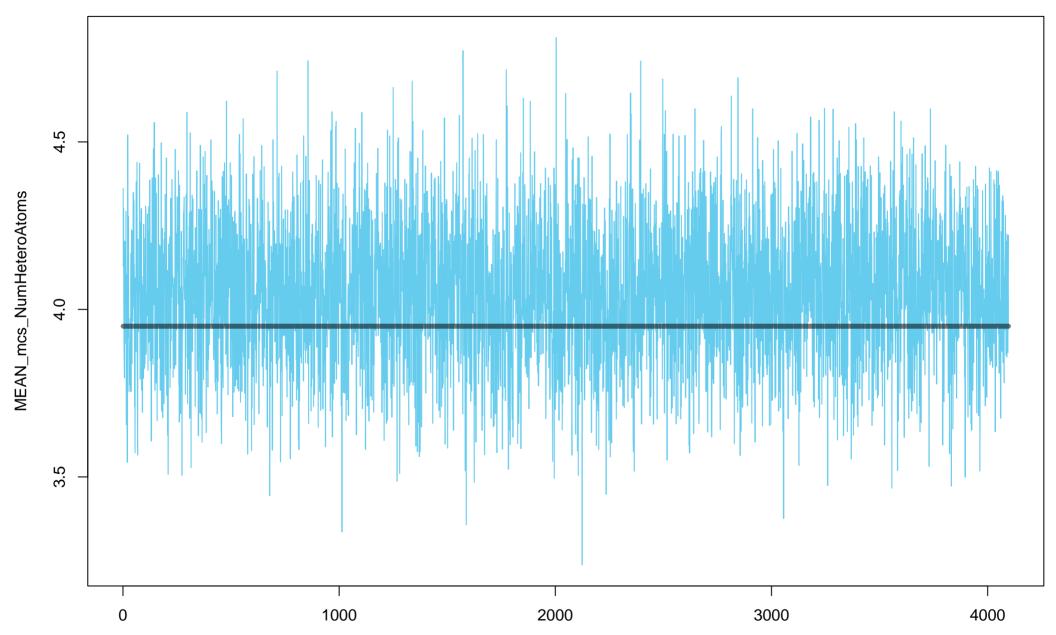
MEAN_log_RMSD ESS = 4070 | BMK = 0.0348 | MCSE(6.27) = 1.6 | stat: FALSE | burn: 0 | rel.err: -0.617



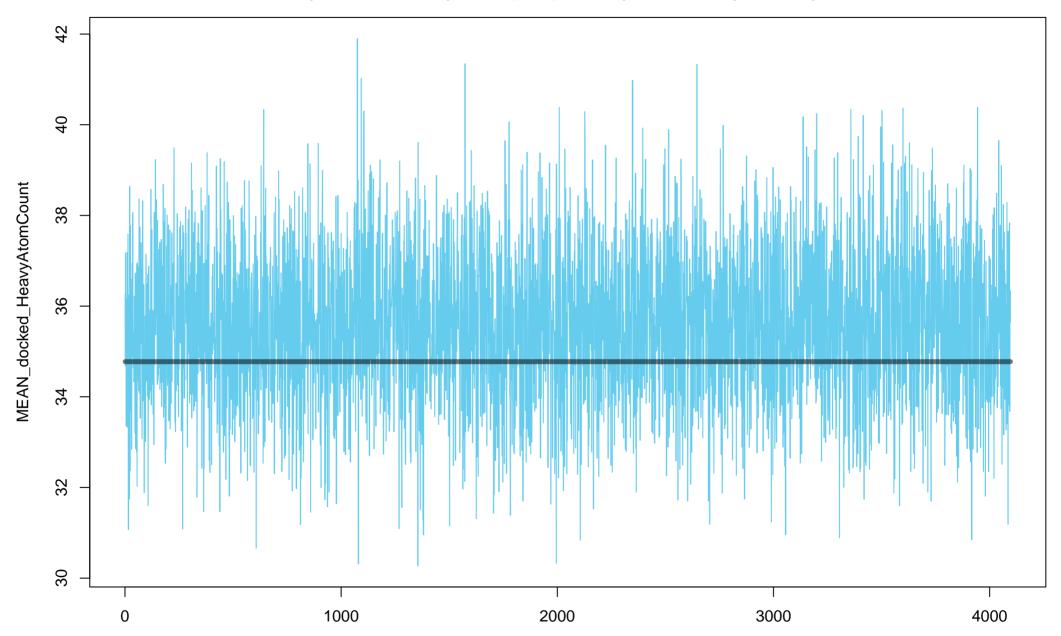
MEAN_log_mcs_unbonded_polar_sasa ESS = 3890 | BMK = 0.0437 | MCSE(6.27) = 1.67 | stat: FALSE | burn: 0 | rel.err: -0.222



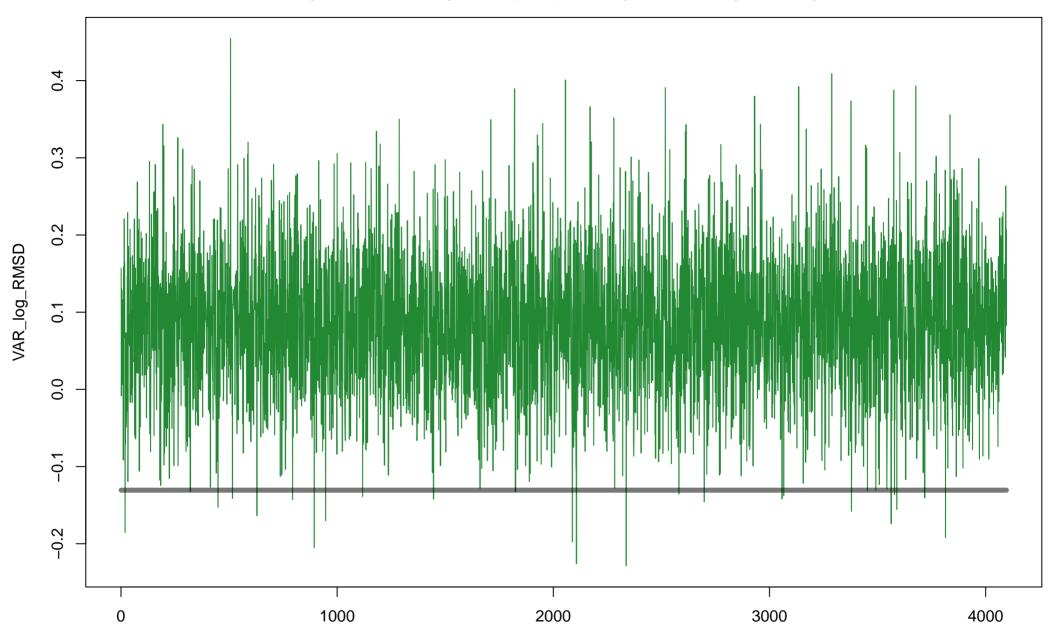
MEAN_mcs_NumHeteroAtoms ESS = 4100 | BMK = 0.031 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0 | rel.err: 0.482



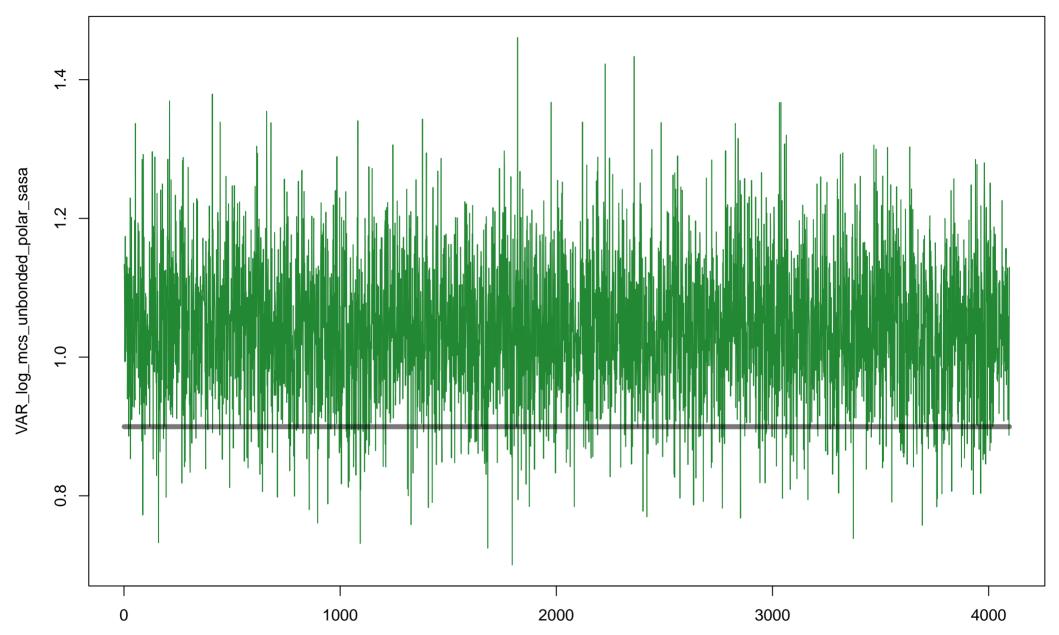
MEAN_docked_HeavyAtomCount ESS = 4100 | BMK = 0.0469 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0 | rel.err: 0.505



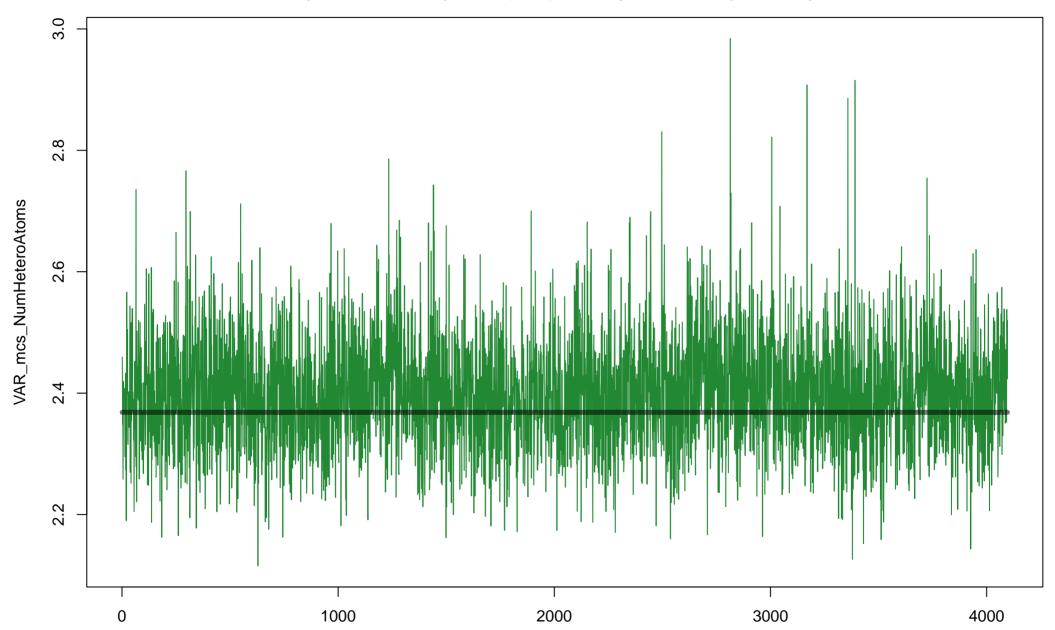
VAR_log_RMSD ESS = 4100 | BMK = 0.0508 | MCSE(6.27) = 1.35 | stat: TRUE | burn: 0 | rel.err: 2.27



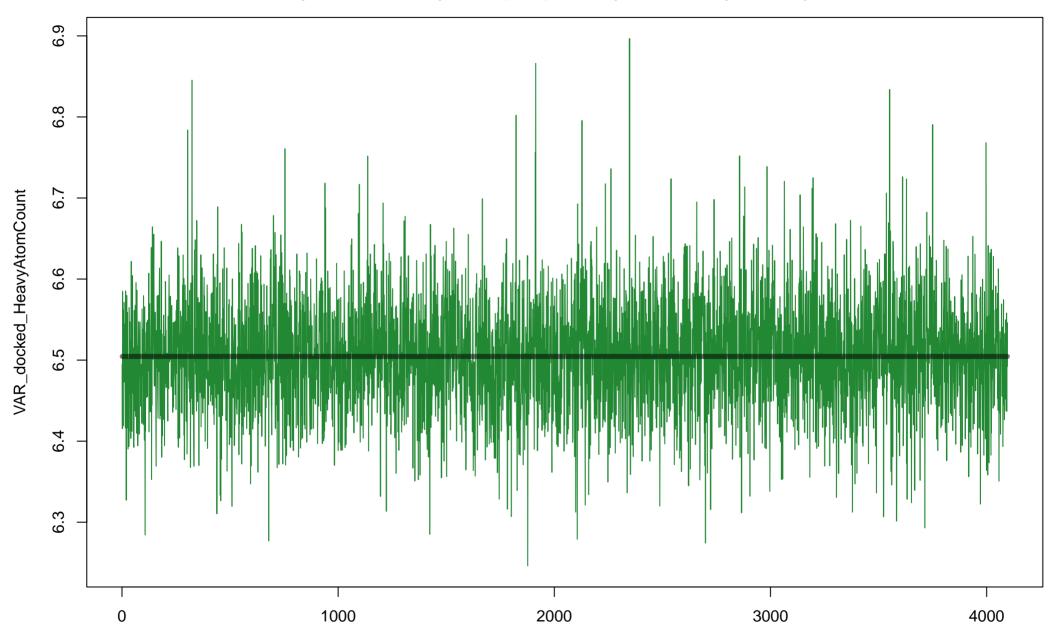
VAR_log_mcs_unbonded_polar_sasa ESS = 3580 | BMK = 0.0421 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: 1.37



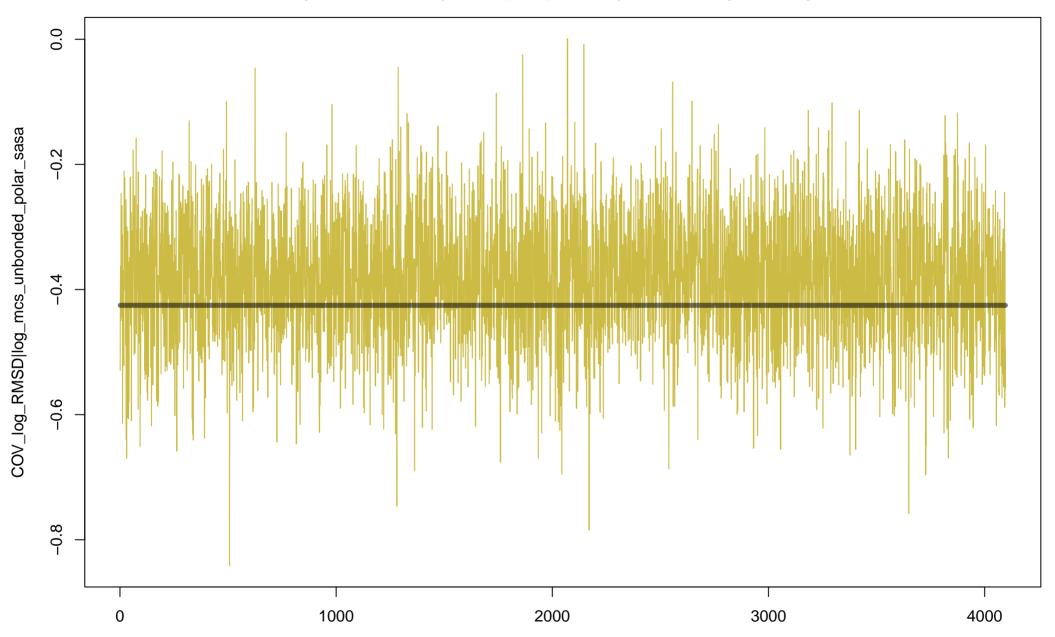
VAR_mcs_NumHeteroAtoms ESS = 2030 | BMK = 0.0511 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 0.398



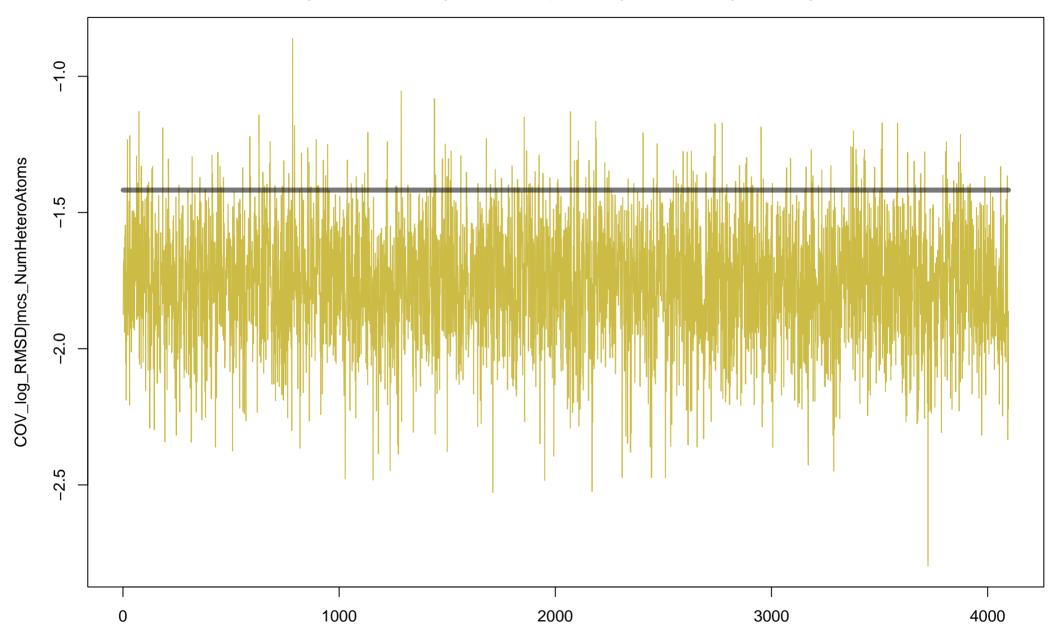
VAR_docked_HeavyAtomCount ESS = 4100 | BMK = 0.0523 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.0565



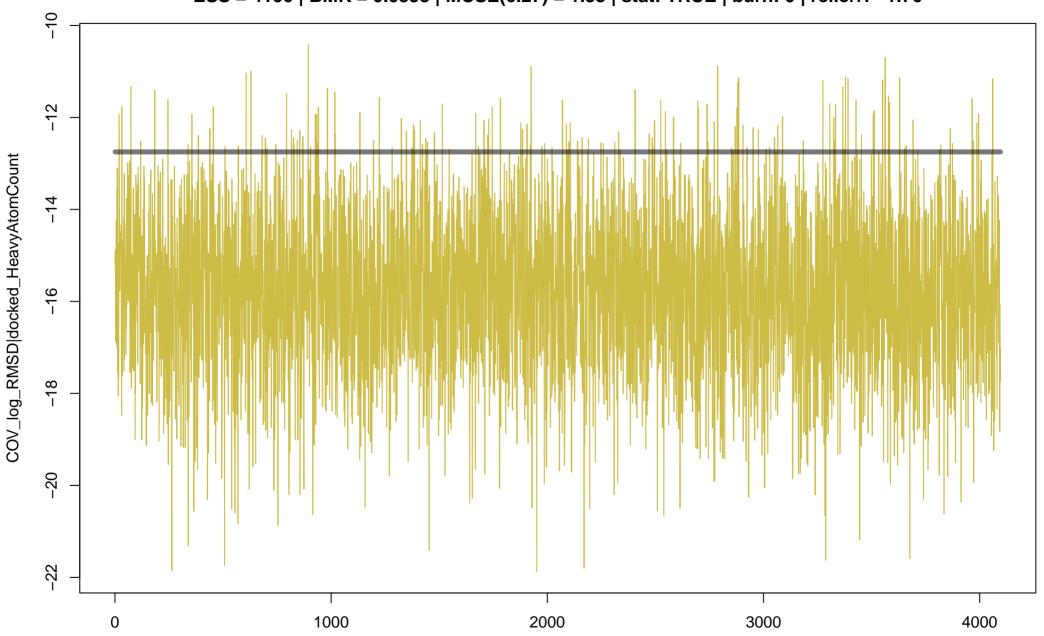
COV_log_RMSD|log_mcs_unbonded_polar_sasa ESS = 3380 | BMK = 0.0286 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: 0.456



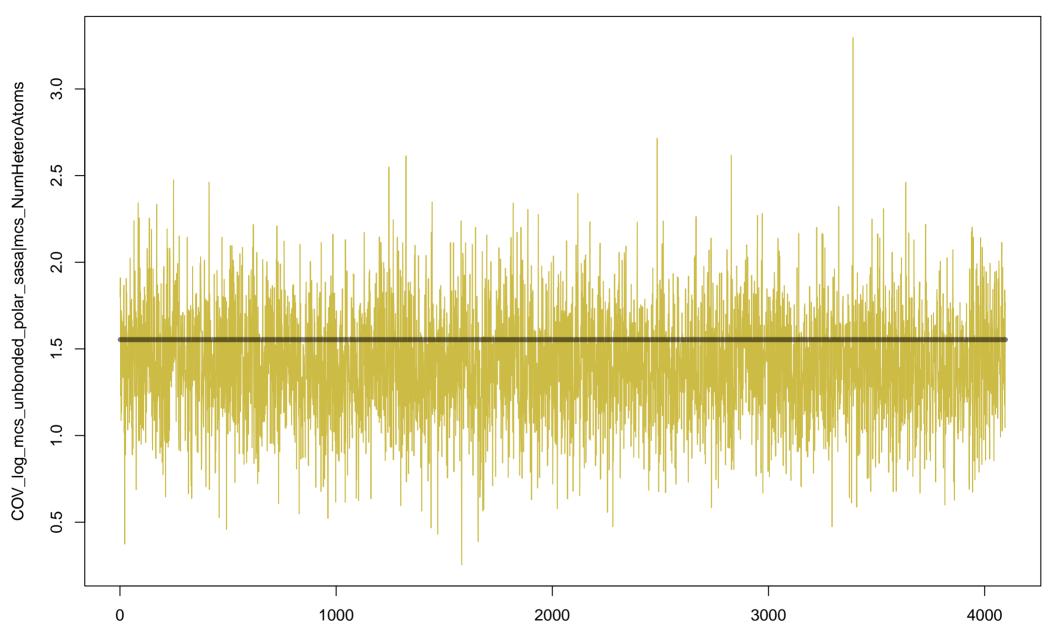
 $COV_log_RMSD|mcs_NumHeteroAtoms \\ ESS = 3580 \mid BMK = 0.0407 \mid MCSE(6.27) = 1.97 \mid stat: TRUE \mid burn: 0 \mid rel.err: -1.57$



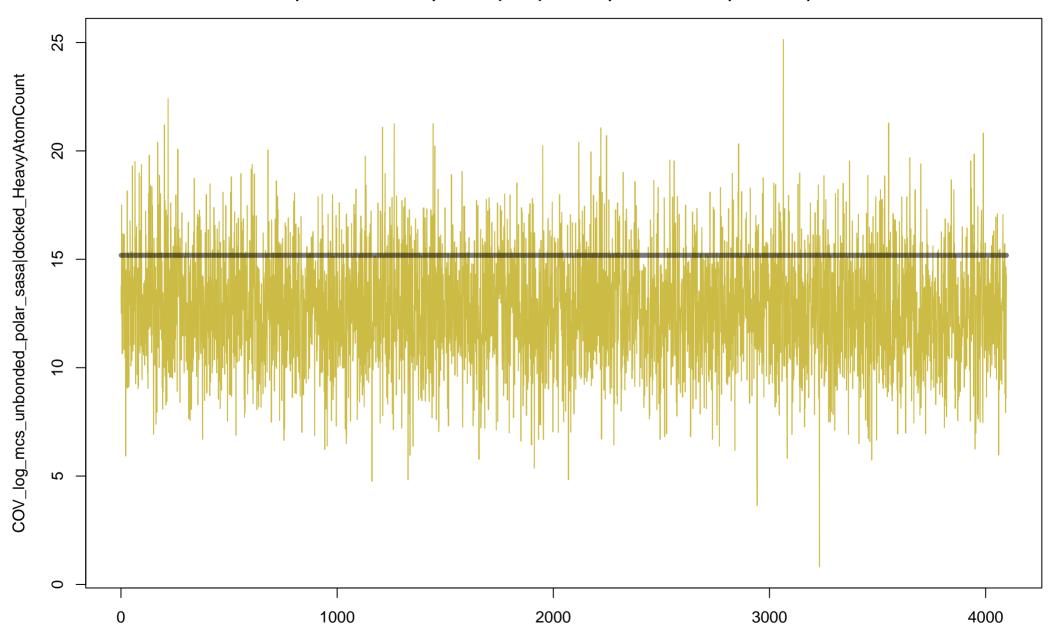
COV_log_RMSD|docked_HeavyAtomCount ESS = 4100 | BMK = 0.0353 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: -1.76



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms ESS = 3660 | BMK = 0.039 | MCSE(6.27) = 1.58 | stat: FALSE | burn: 0 | rel.err: -0.452



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount ESS = 3820 | BMK = 0.0383 | MCSE(6.27) = 1.64 | stat: FALSE | burn: 0 | rel.err: -0.957



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount ESS = 4100 | BMK = 0.0392 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 0.478

