-- STATS maxD --

min ESS = 86.0221147575997

max BMK = 0.139986662190434

max MCSE = 8.08471263084366

all stationary: TRUE

burn: 0

max rel.err.: 2.20020726187788

-- STATS 1D --

min ESS = 1692.35601899538

max BMK = 0.0673295720463373

 $max\ MCSE = 2.74488492605211$ 

all stationary: TRUE

burn: 0

max rel.err.: 2.25180864667938

-- STATS 2D --

min ESS = 1785.58446483707

max BMK = 0.0573894307874708

max MCSE = 2.78498209925673

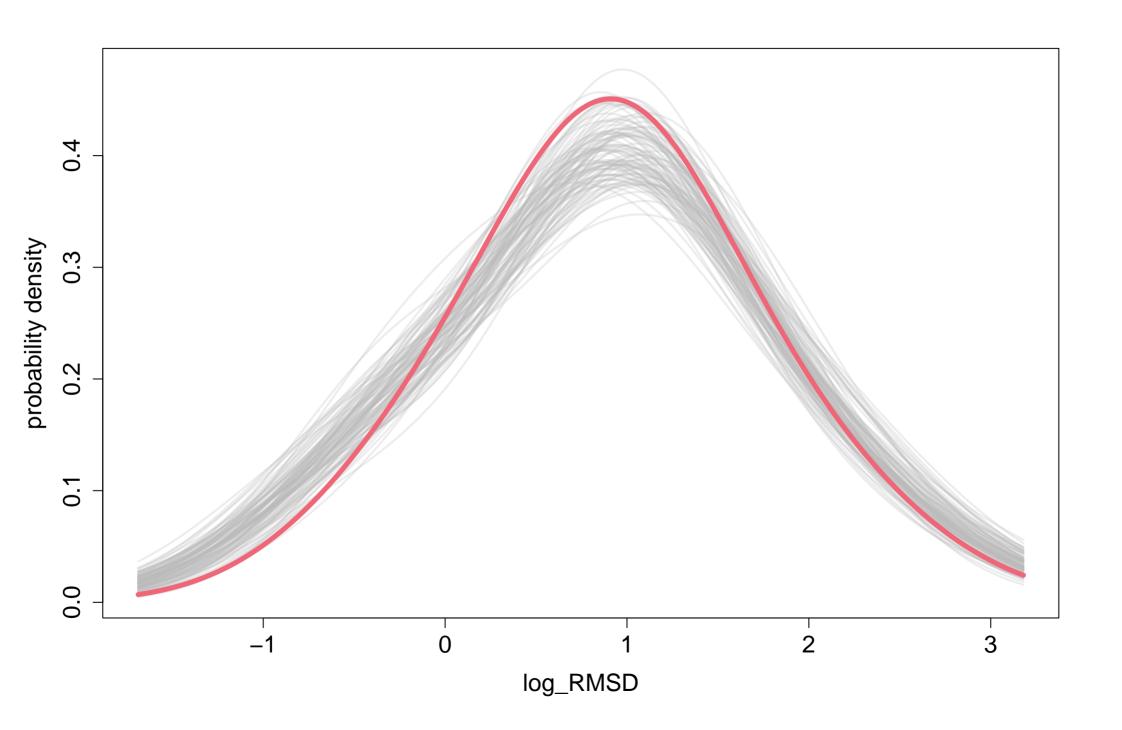
all stationary: TRUE

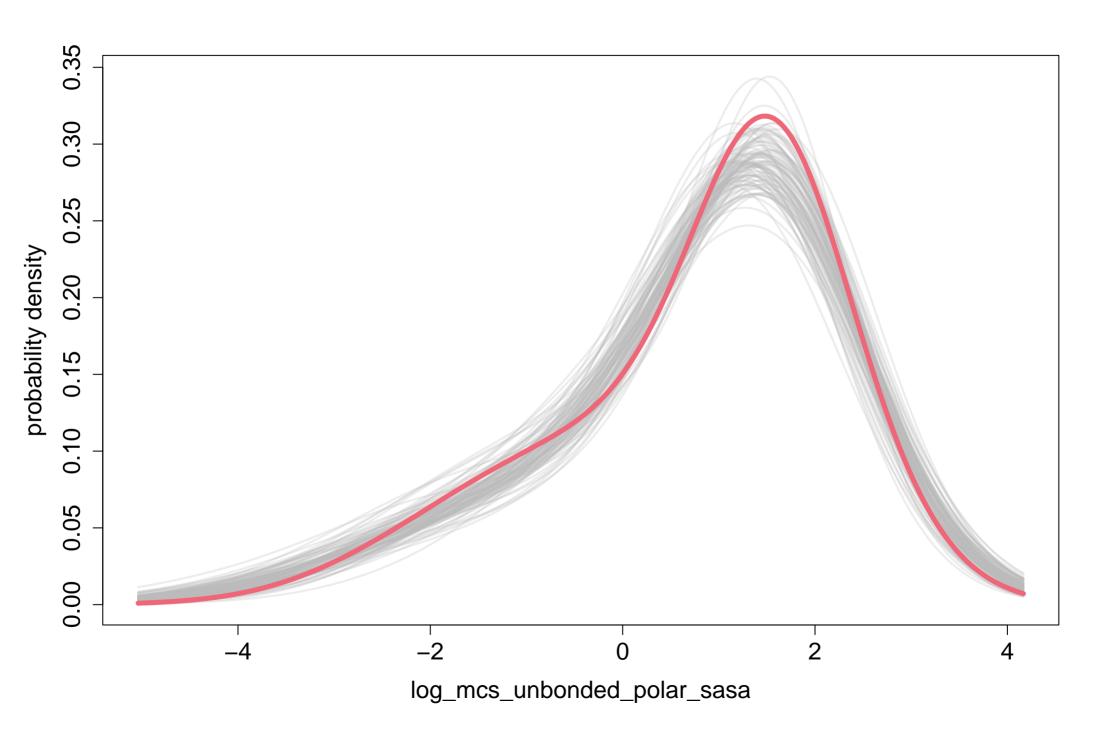
burn: 0

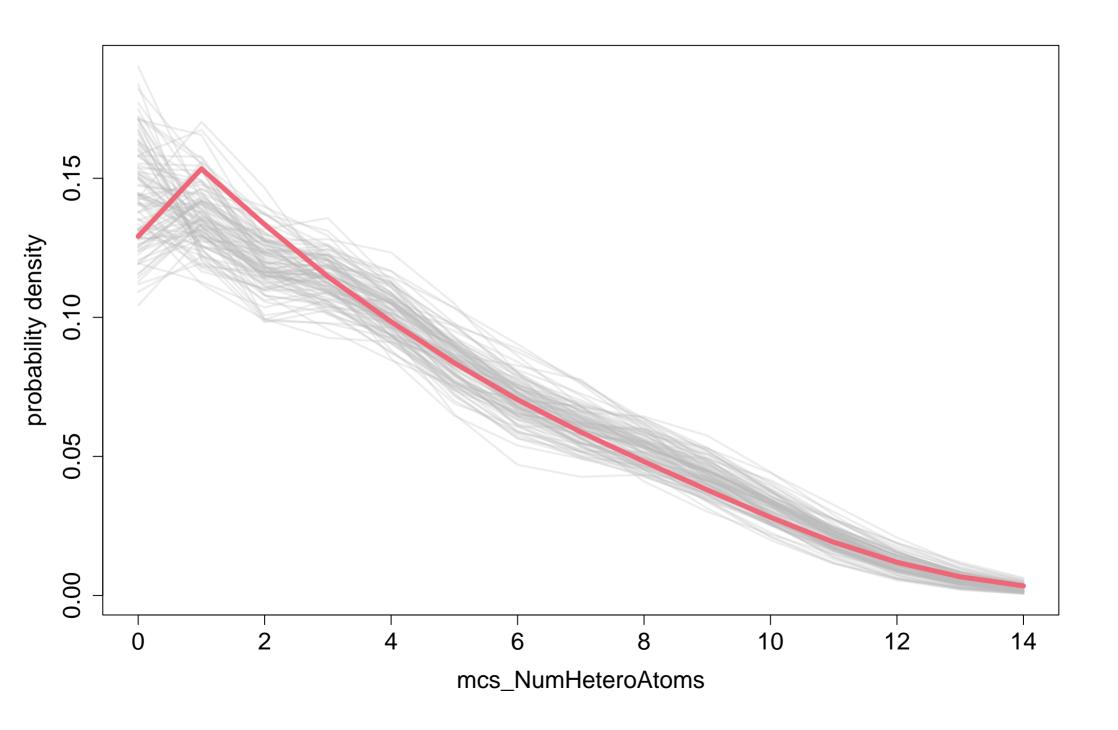
max rel.err.: 1.70997539950496

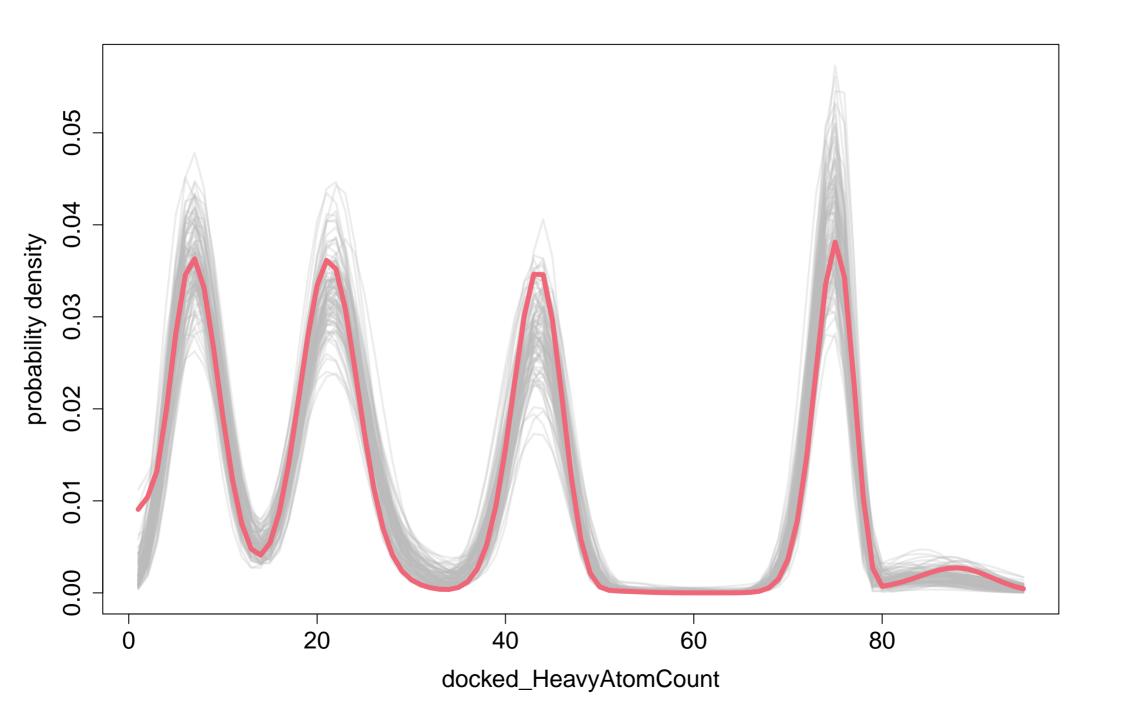
Occupied clusters: 9 of 16

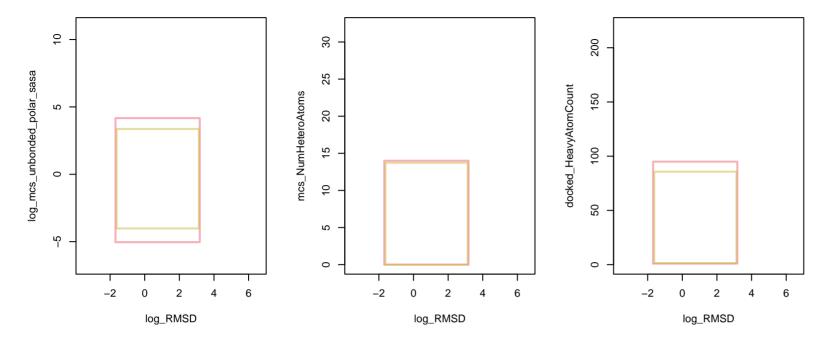
LL: -2158.5746193312 sd: 6.62422812286771





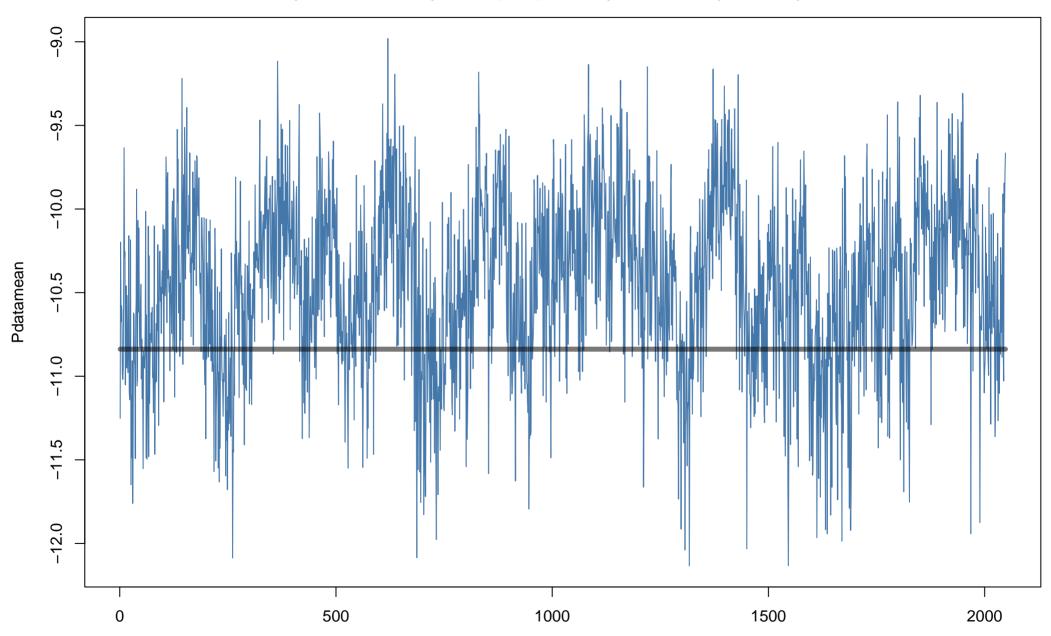




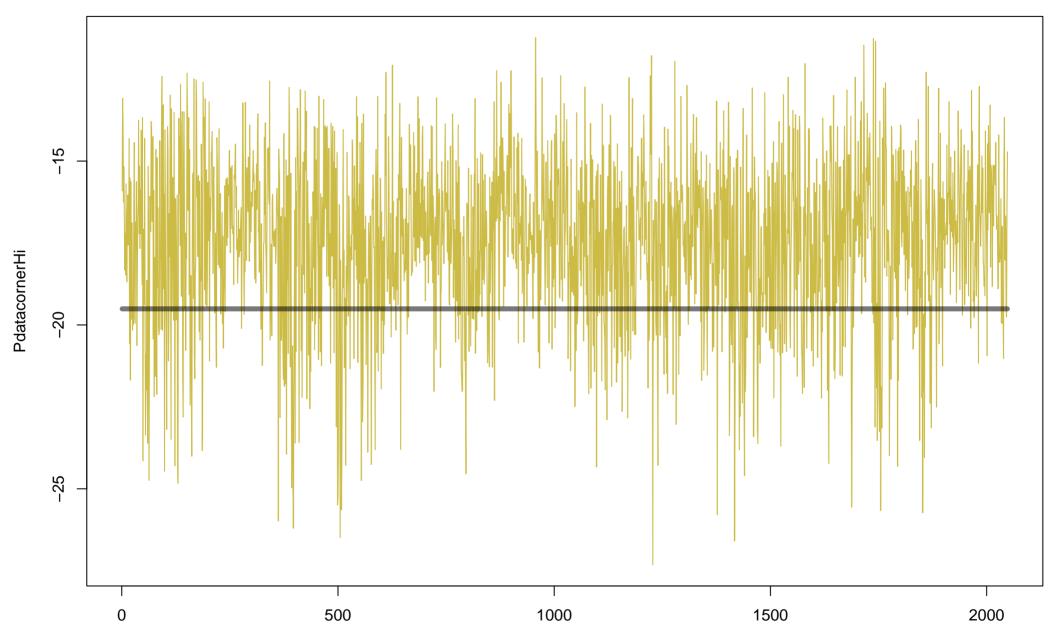


Pdatamean

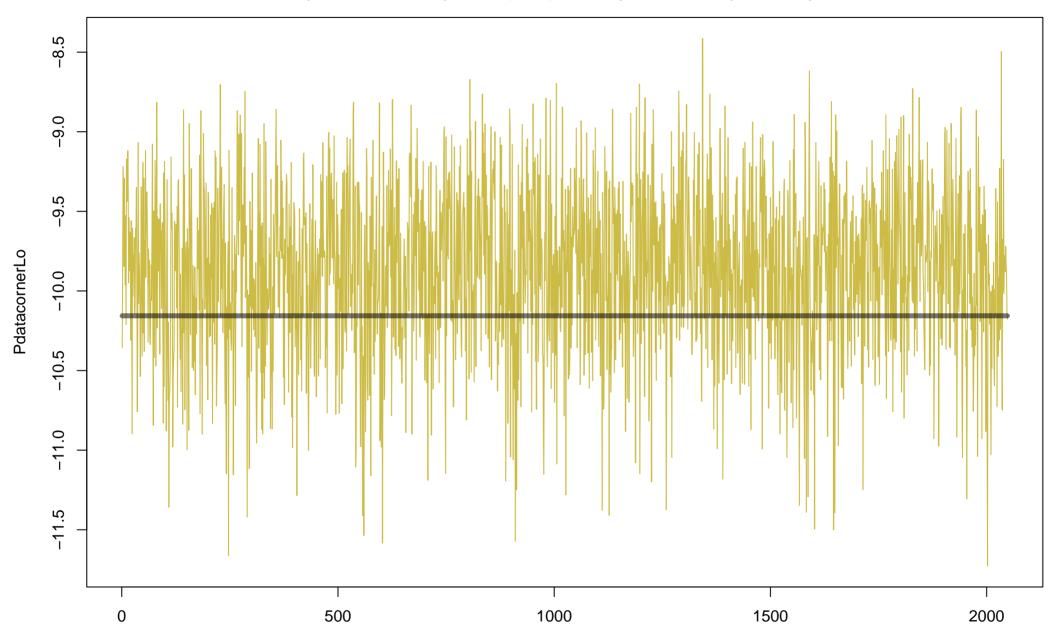
ESS = 86 | BMK = 0.0607 | MCSE(6.27) = 8.08 | stat: TRUE | burn: 0 | rel.err: 0.795



PdatacornerHi
ESS = 977 | BMK = 0.14 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.304

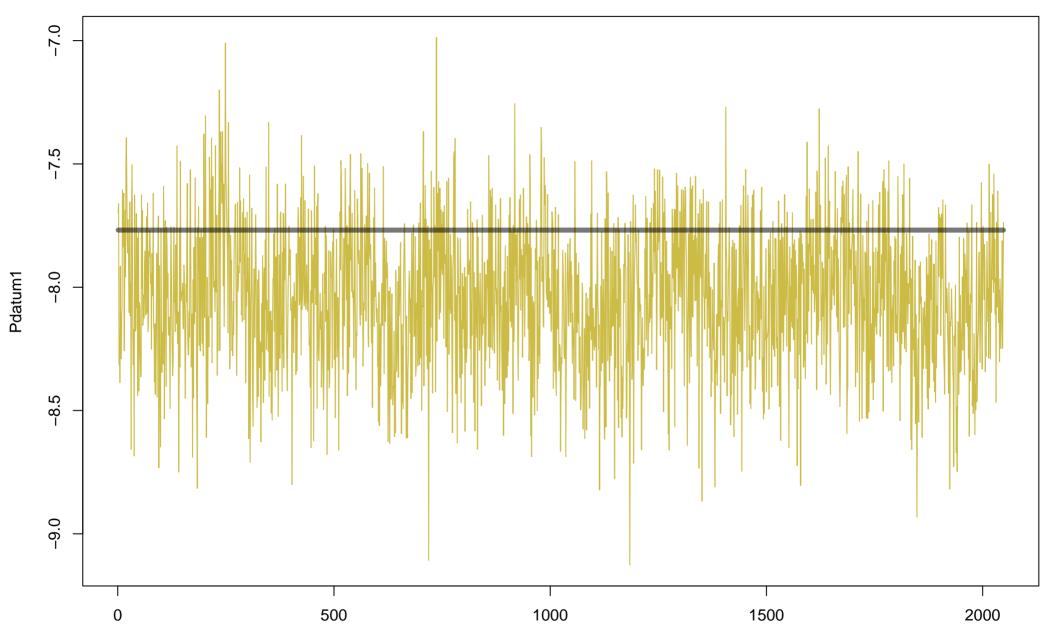


PdatacornerLo
ESS = 1760 | BMK = 0.0506 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.685

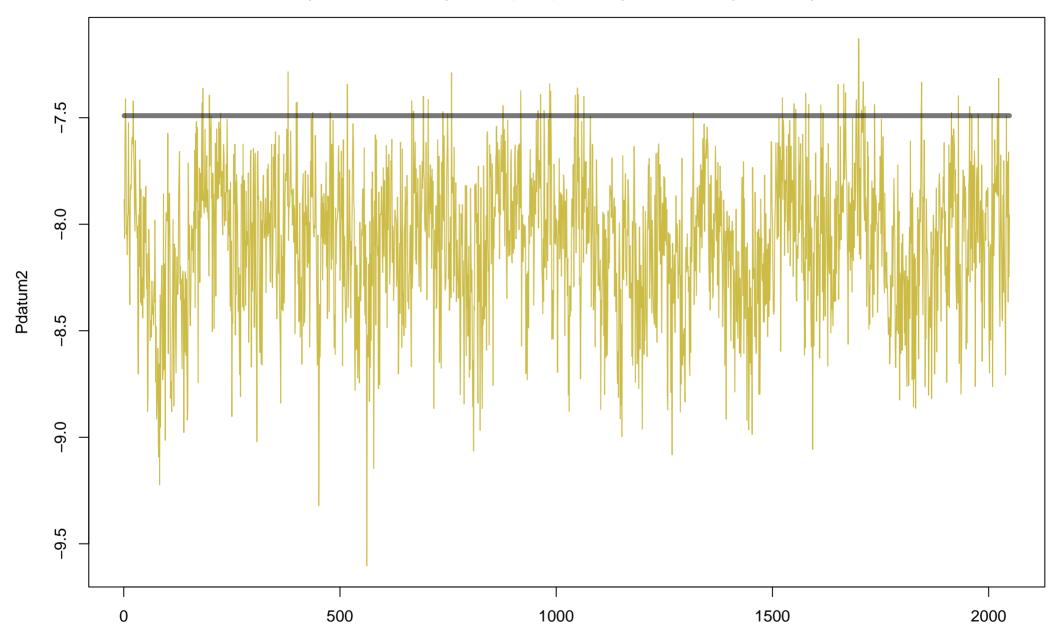


Pdatum1

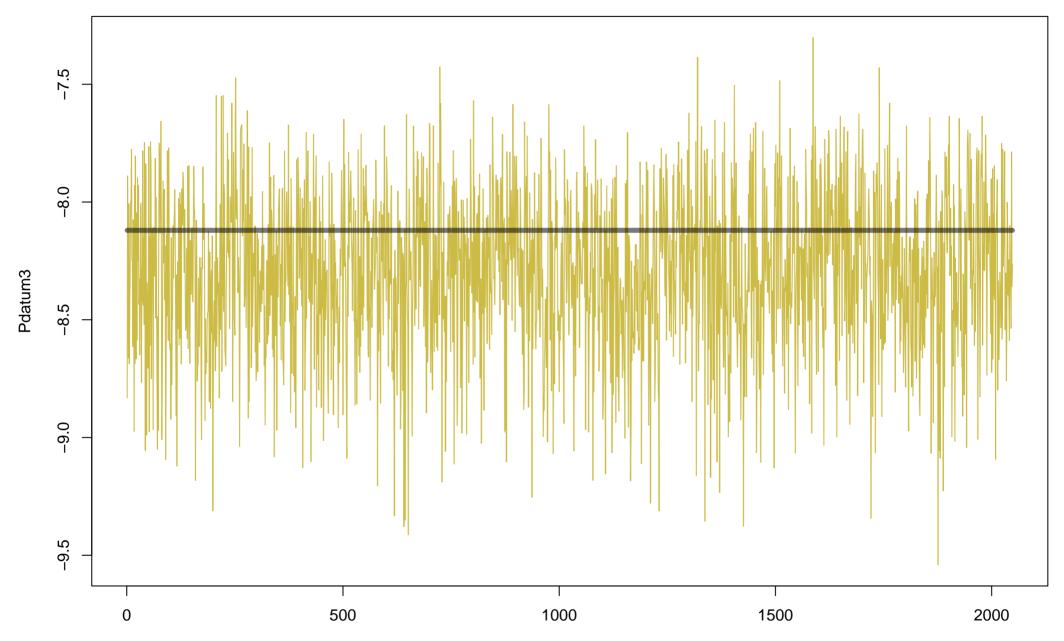
ESS = 408 | BMK = 0.0719 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0 | rel.err: -0.935



Pdatum2 ESS = 262 | BMK = 0.0656 | MCSE(6.27) = 6.32 | stat: TRUE | burn: 0 | rel.err: -2.2

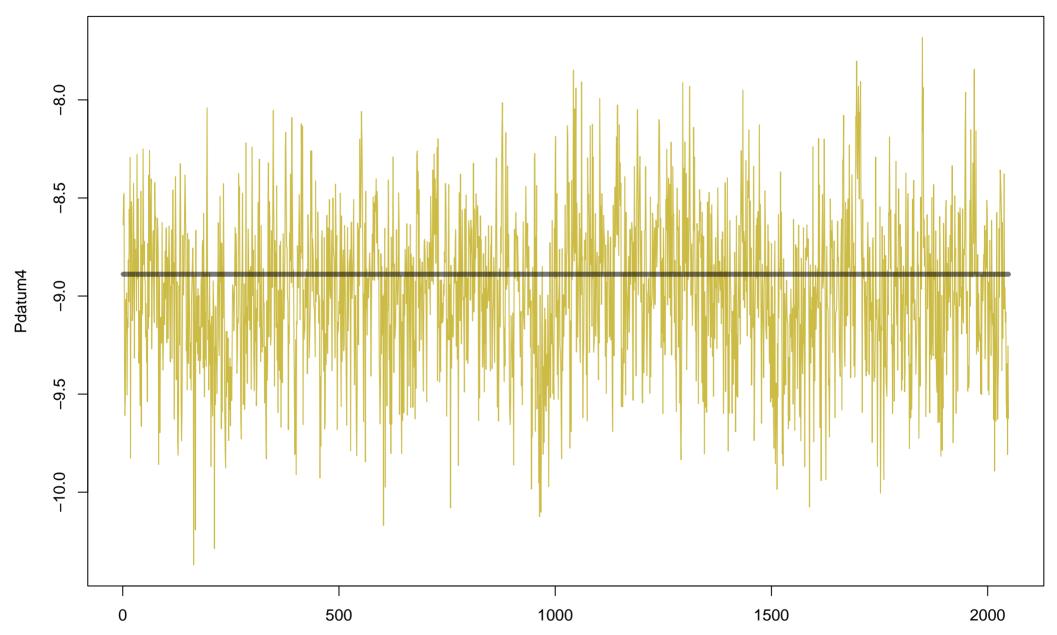


Pdatum3 ESS = 1160 | BMK = 0.0445 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: -0.398



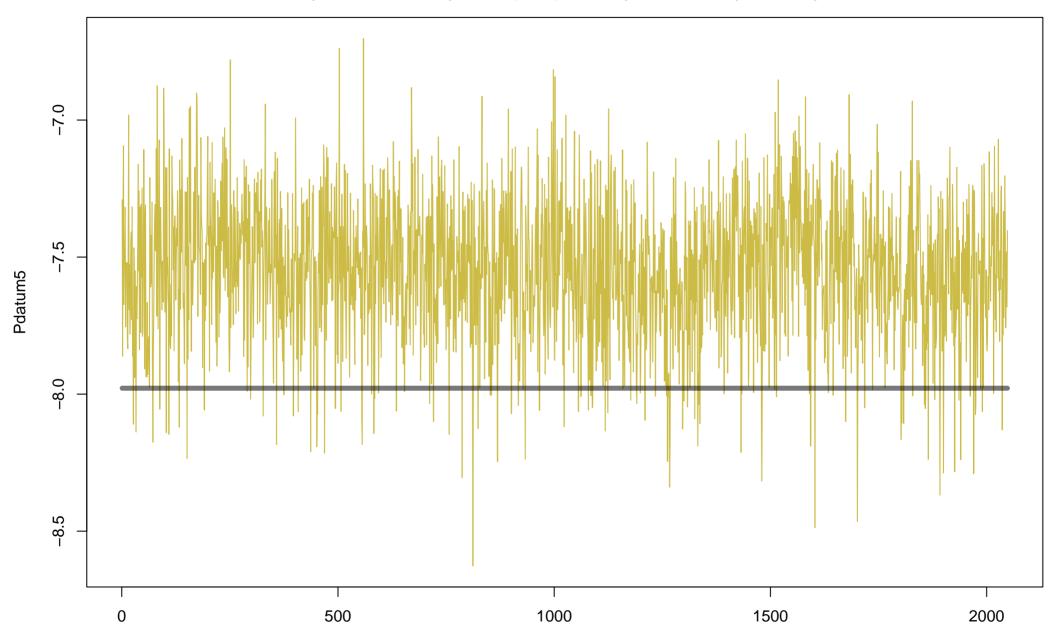
Pdatum4

ESS = 621 | BMK = 0.0917 | MCSE(6.27) = 4.58 | stat: TRUE | burn: 0 | rel.err: -0.0399

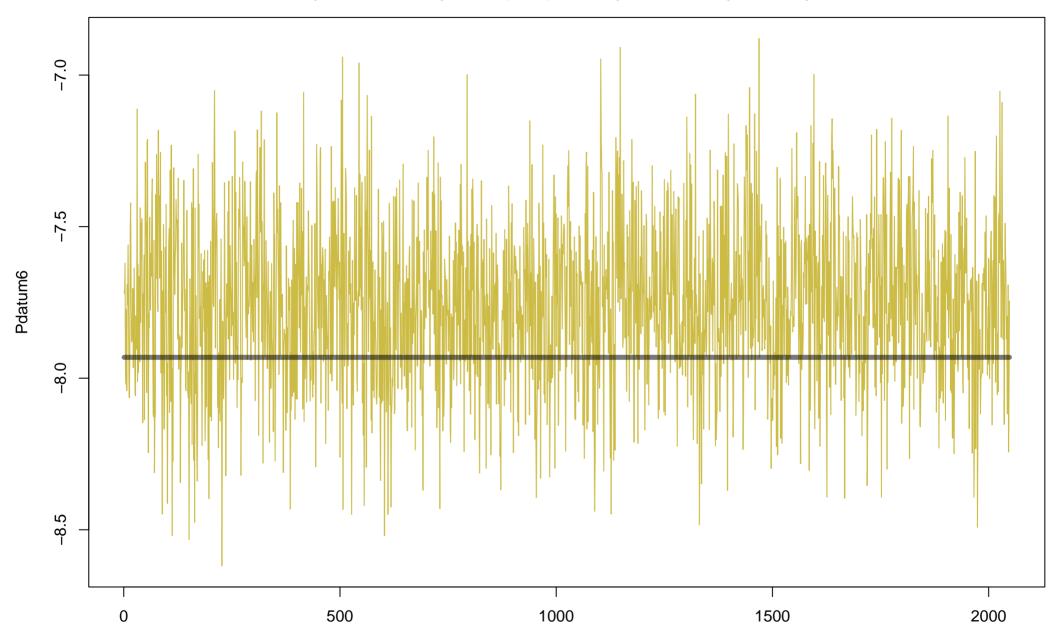


Pdatum5

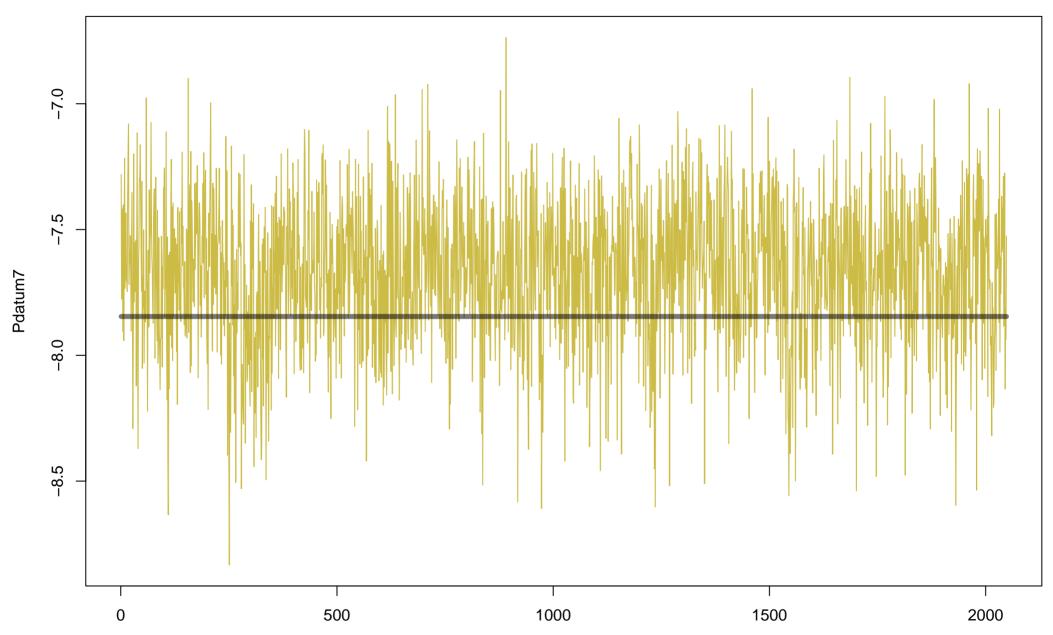
ESS = 1350 | BMK = 0.0648 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: 1.46



Pdatum6 ESS = 1140 | BMK = 0.054 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | rel.err: 0.703

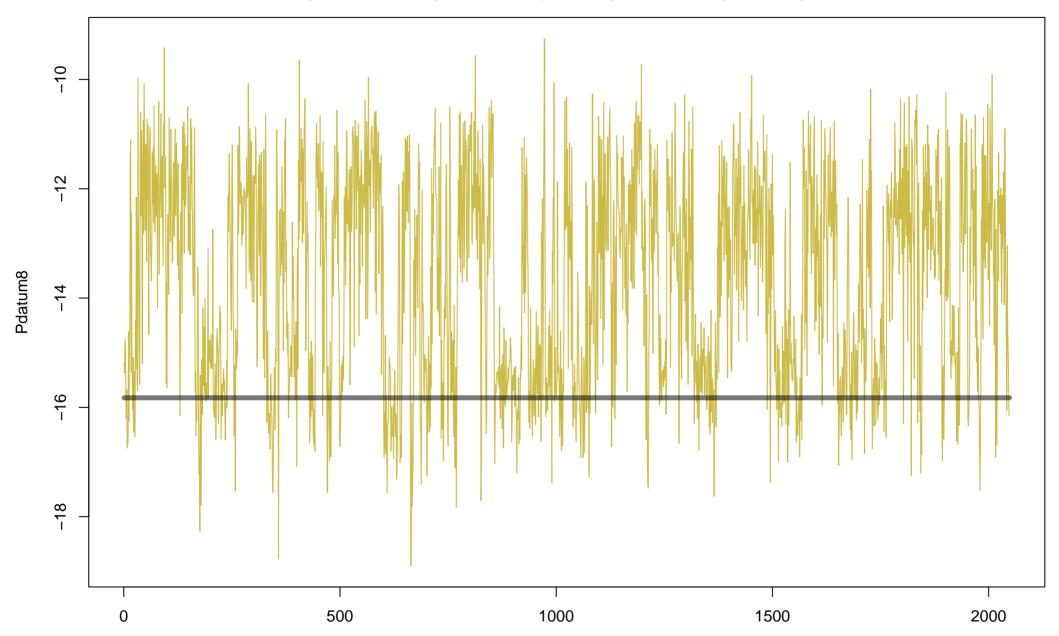


Pdatum7
ESS = 925 | BMK = 0.0439 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | rel.err: 0.687

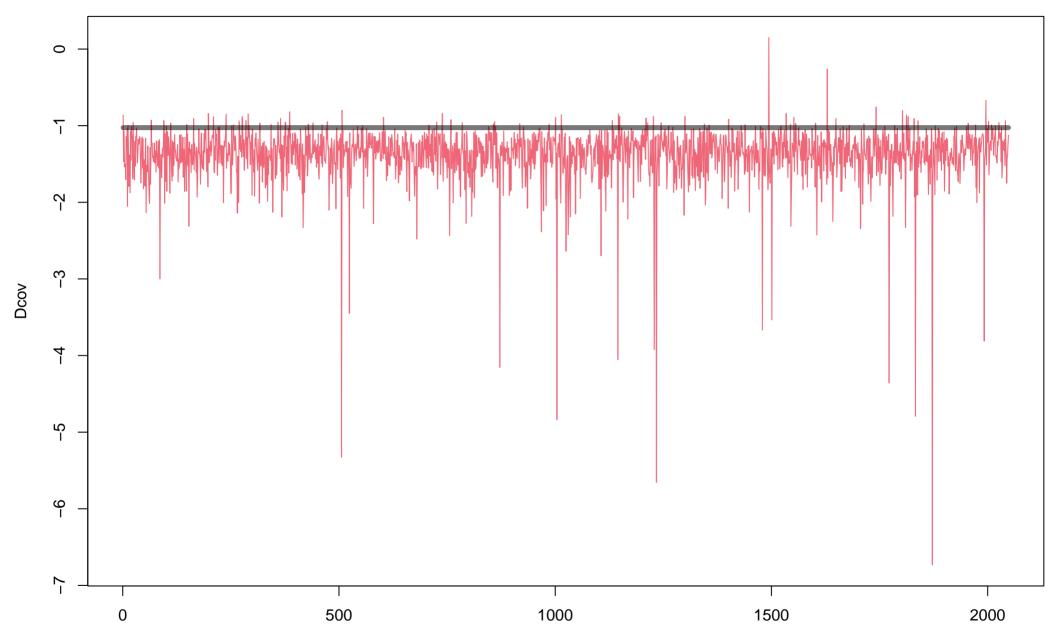


Pdatum8

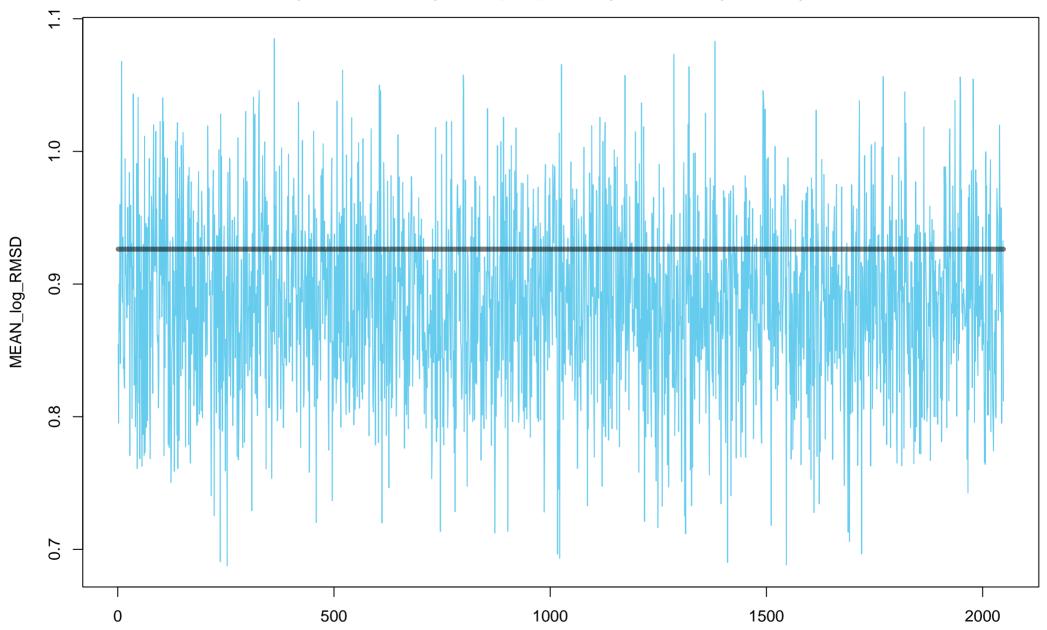
ESS = 407 | BMK = 0.102 | MCSE(6.27) = 4.99 | stat: TRUE | burn: 0 | rel.err: 0.578



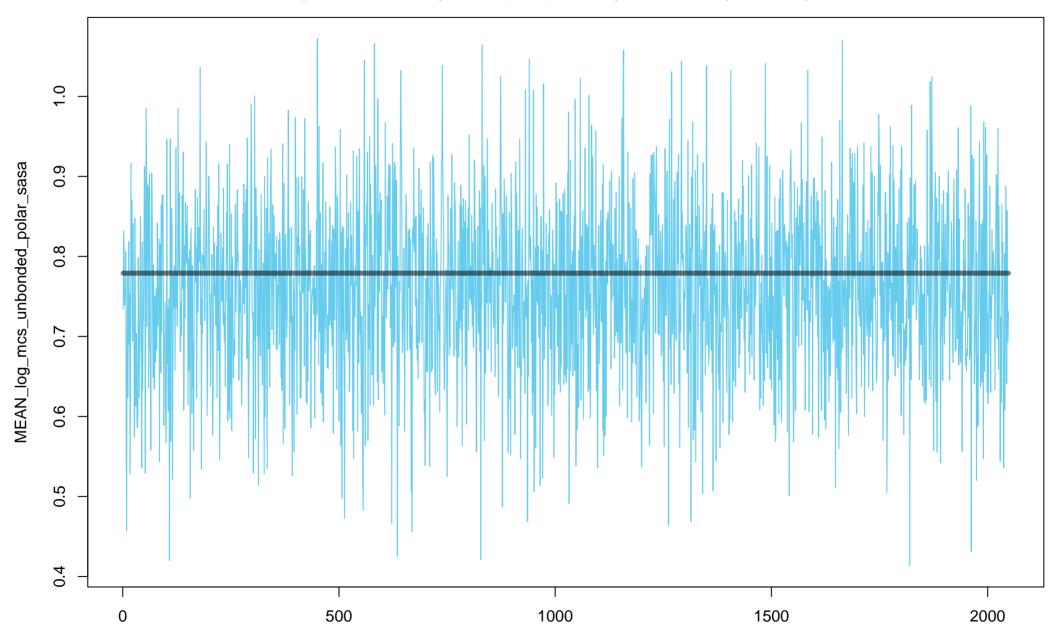
Dcov ESS = 1770 | BMK = 0.0579 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 1.33



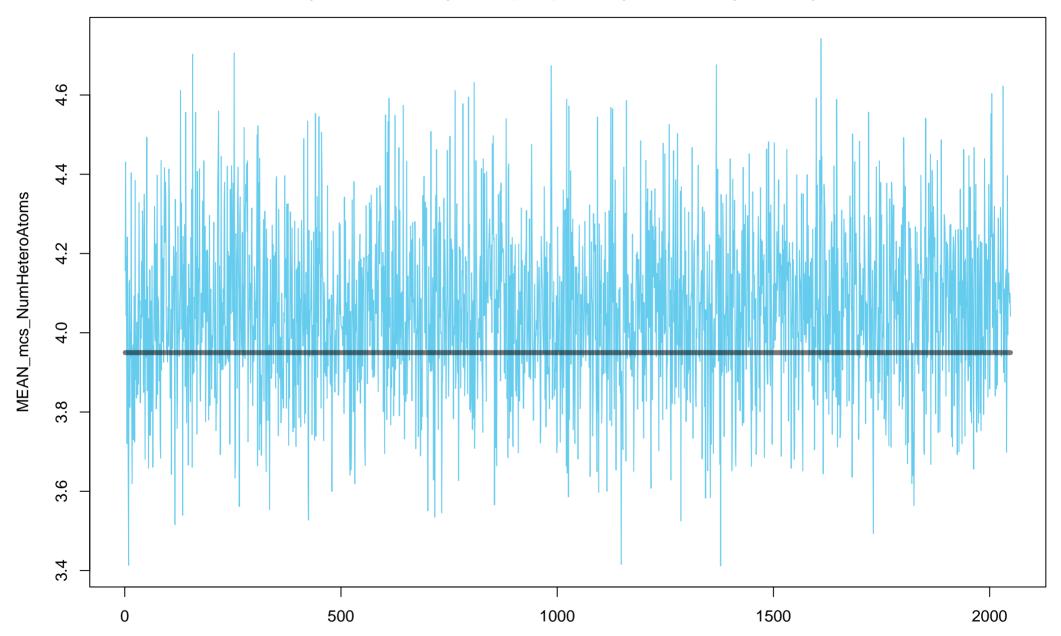
MEAN\_log\_RMSD ESS = 2050 | BMK = 0.0535 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: -0.604



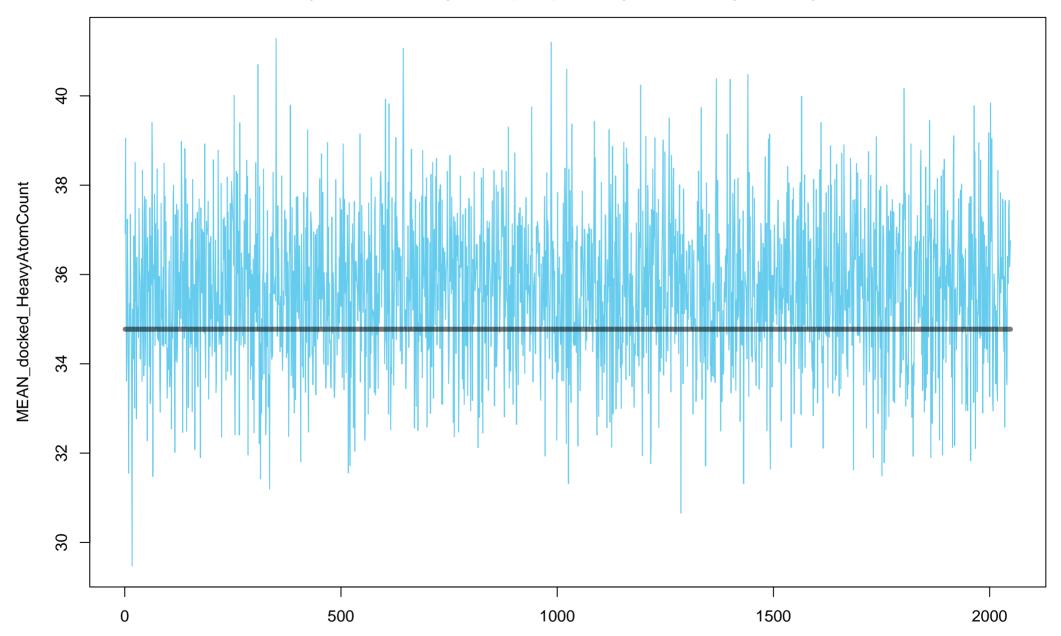
MEAN\_log\_mcs\_unbonded\_polar\_sasa ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: -0.197



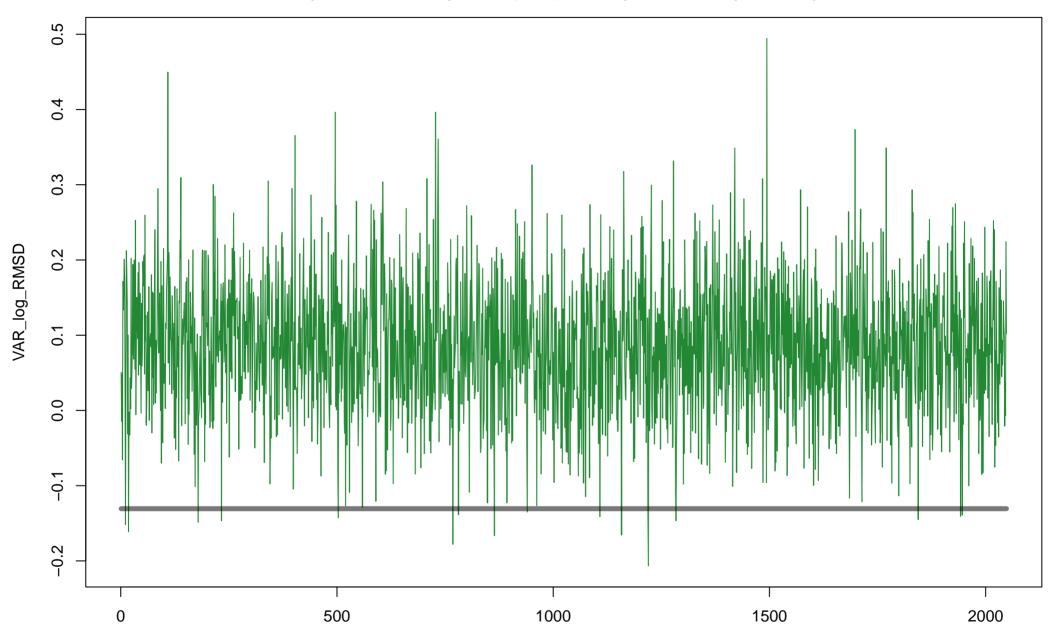
MEAN\_mcs\_NumHeteroAtoms ESS = 2050 | BMK = 0.0412 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: 0.521



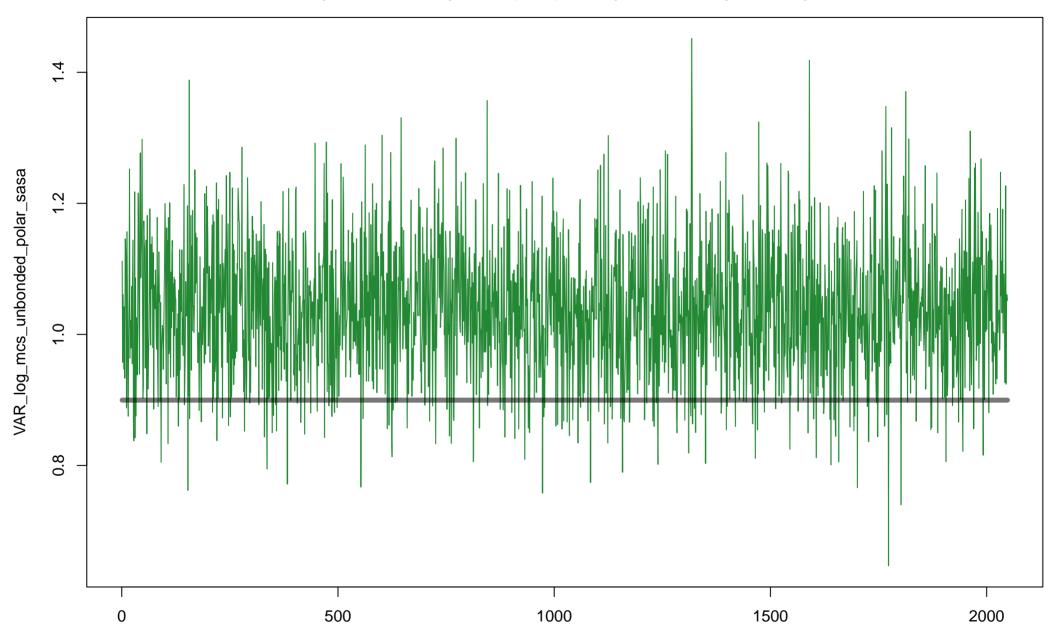
MEAN\_docked\_HeavyAtomCount ESS = 2050 | BMK = 0.0422 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: 0.542



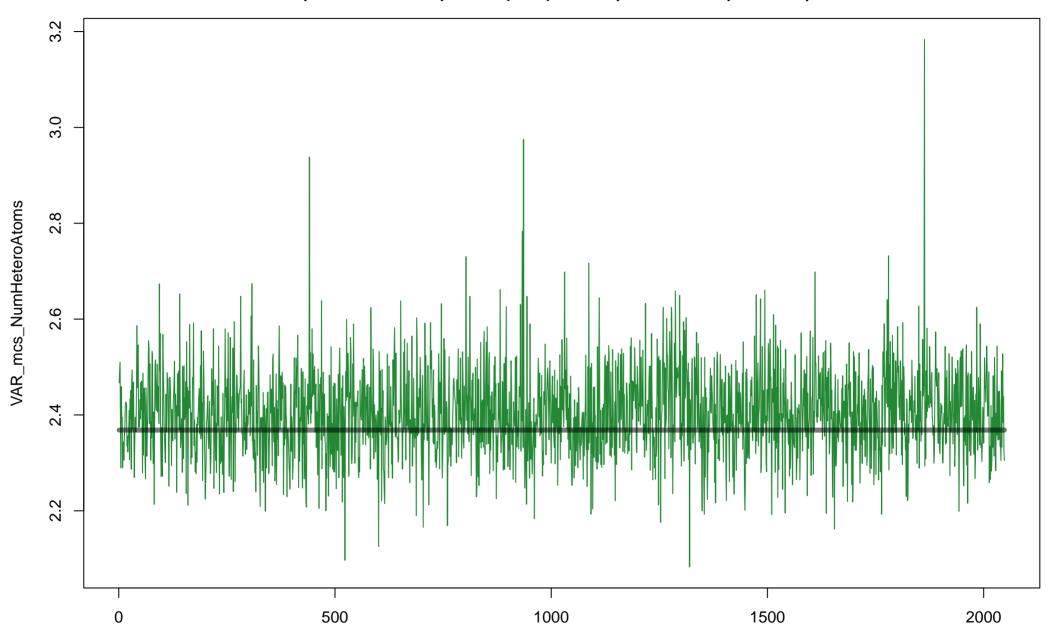
VAR\_log\_RMSD ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: 2.25



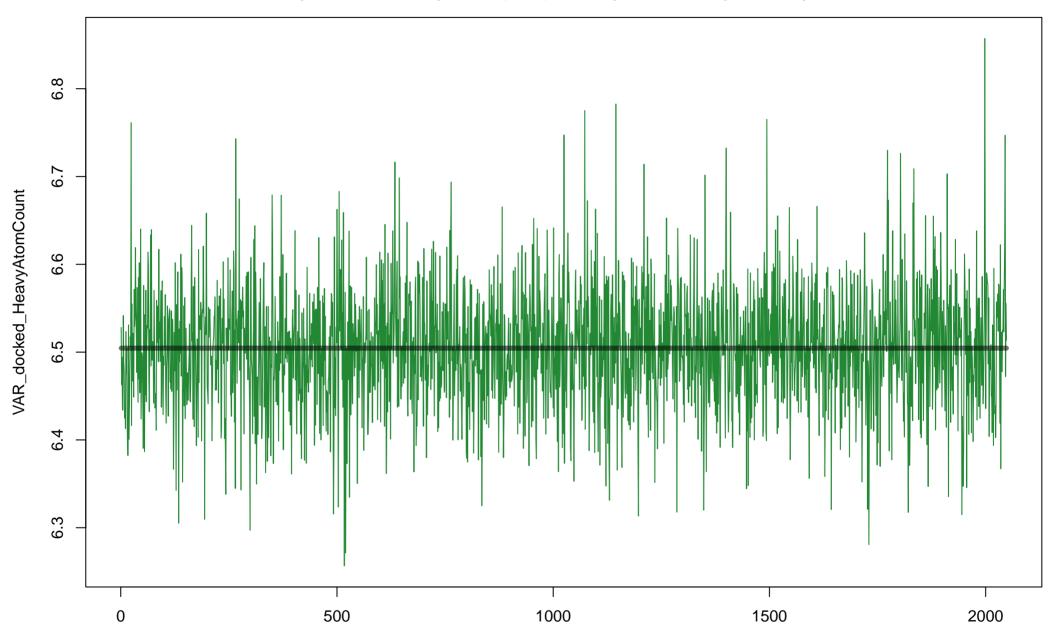
VAR\_log\_mcs\_unbonded\_polar\_sasa ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: 1.31



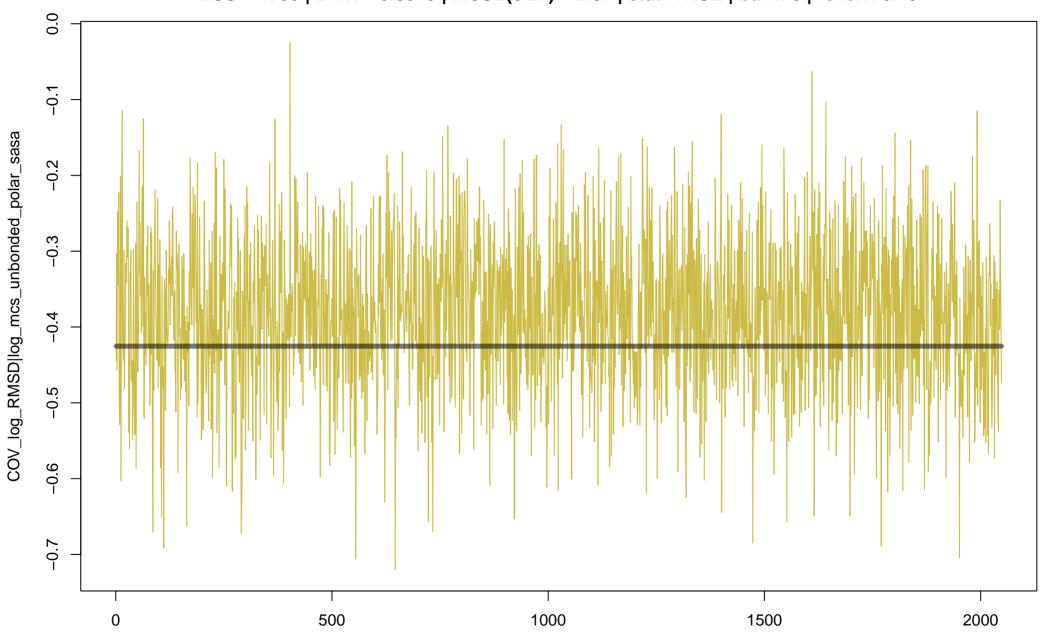
VAR\_mcs\_NumHeteroAtoms ESS = 1690 | BMK = 0.0673 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: 0.403



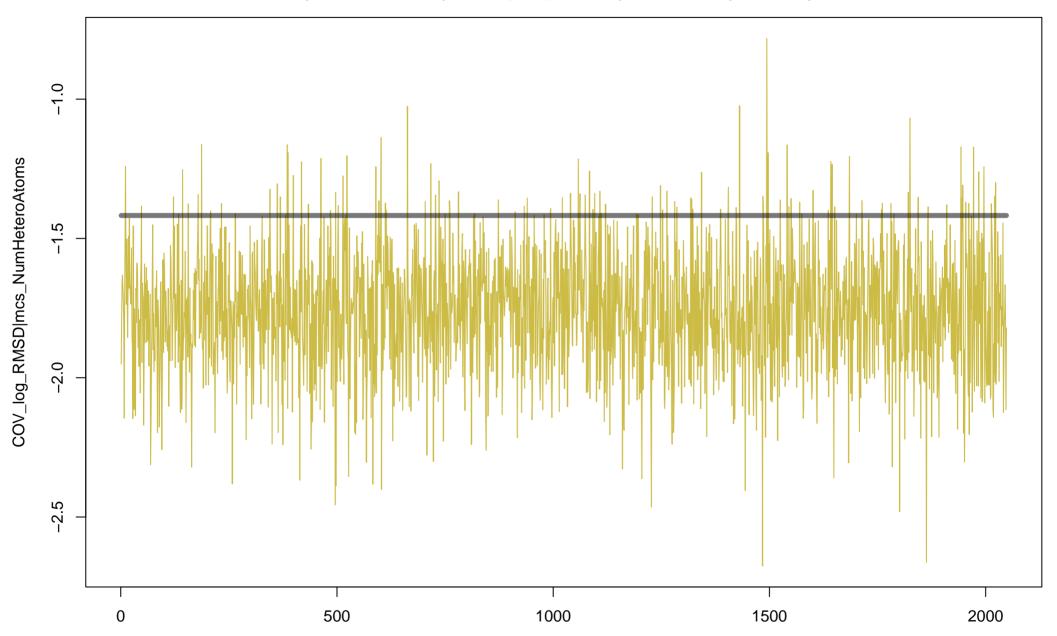
VAR\_docked\_HeavyAtomCount ESS = 2050 | BMK = 0.0589 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.0354



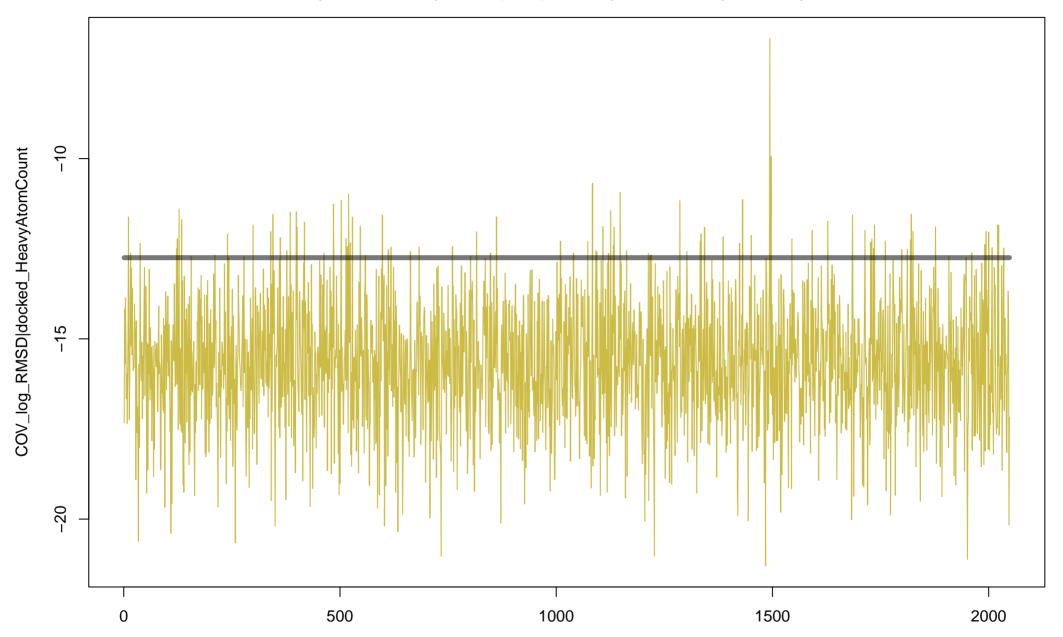
COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa ESS = 1790 | BMK = 0.0319 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 0.45



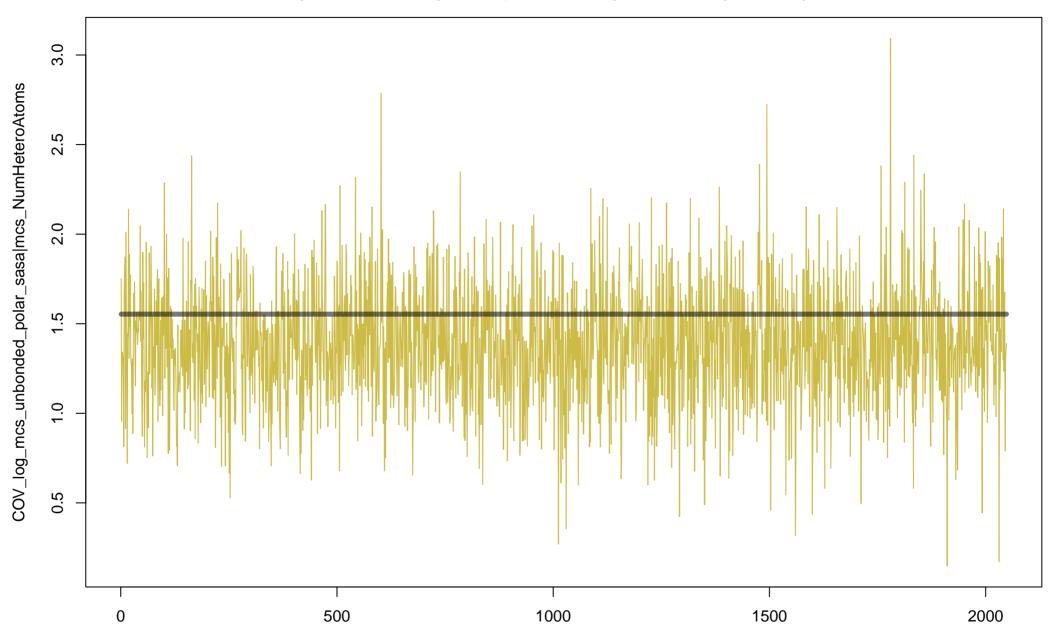
COV\_log\_RMSD|mcs\_NumHeteroAtoms ESS = 1920 | BMK = 0.0574 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: -1.57



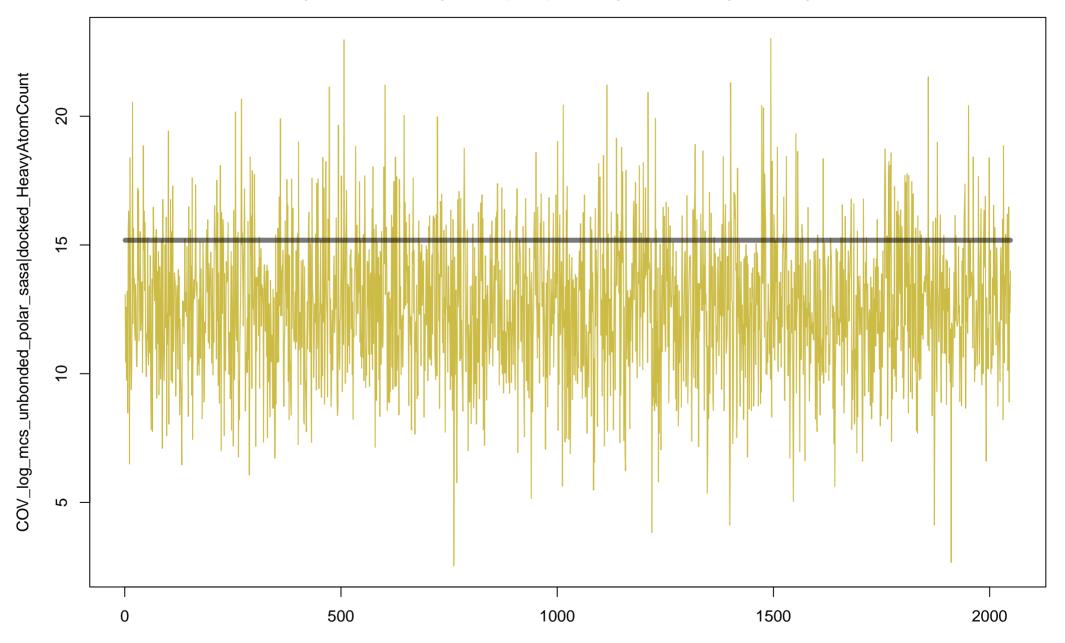
COV\_log\_RMSD|docked\_HeavyAtomCount ESS = 2050 | BMK = 0.04 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: -1.71



COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms ESS = 1890 | BMK = 0.0554 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: -0.498



COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount ESS = 1890 | BMK = 0.0405 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: -0.941



COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount ESS = 2050 | BMK = 0.0561 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.482

