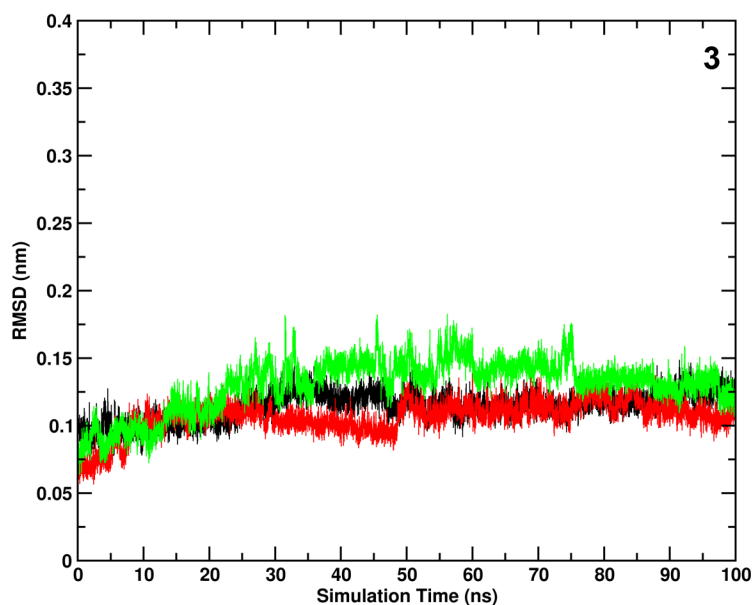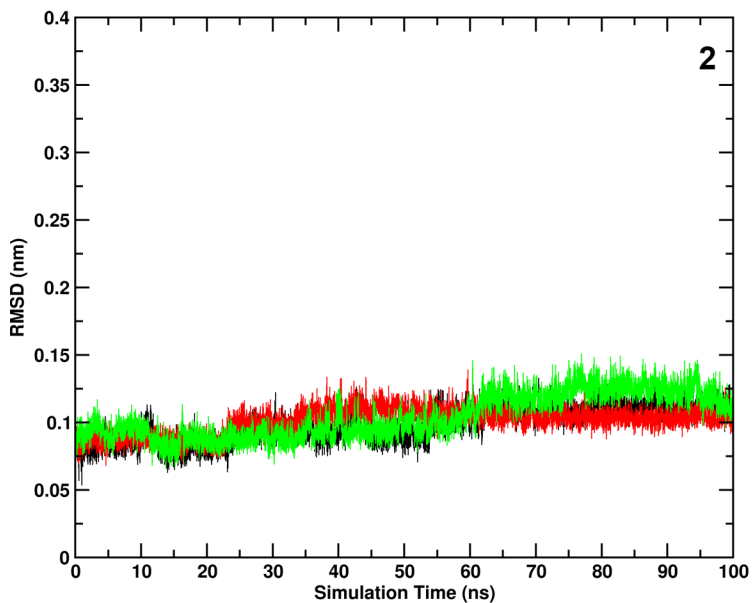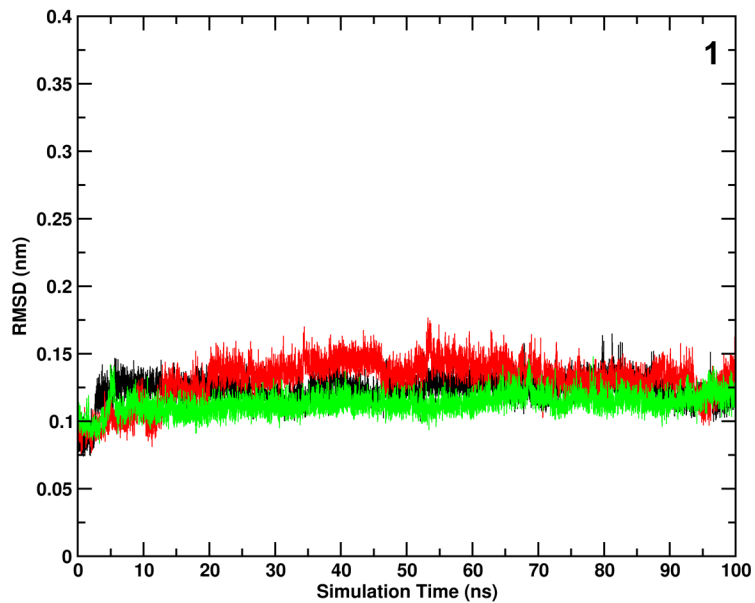# Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms of N2 Systems

All values relative to post-minimization structre (pre-equilibration)
common to the triplicate runs.
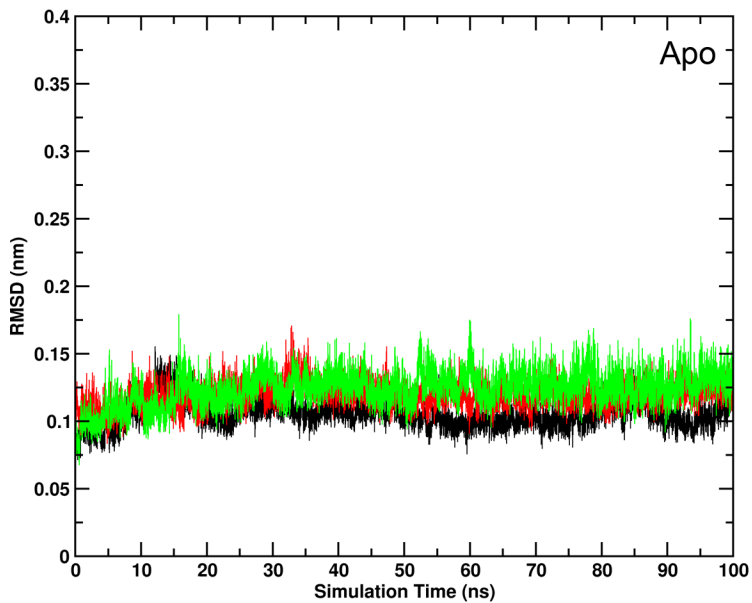
Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms of N2 Systems

All values relative to post-minimization structre (pre-equilibration)
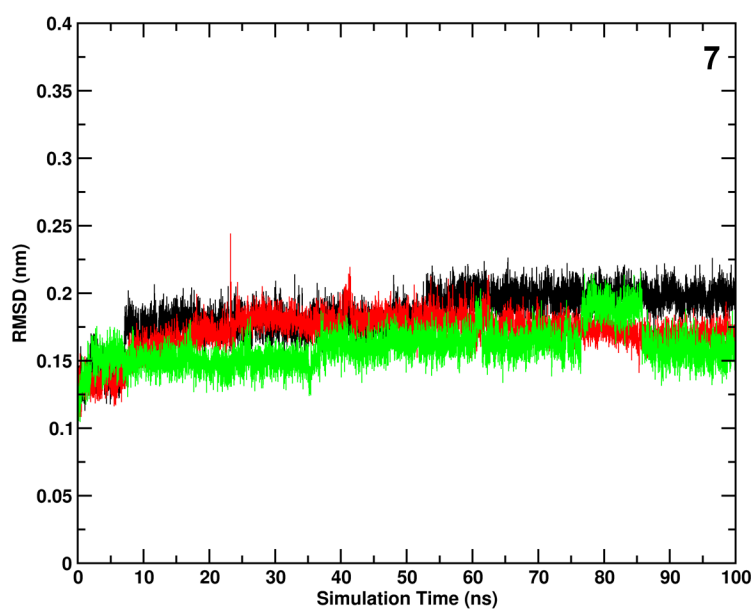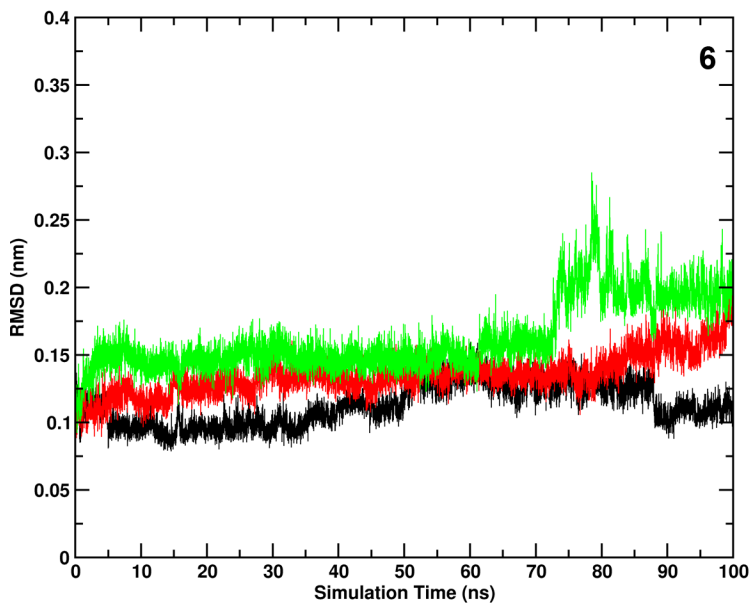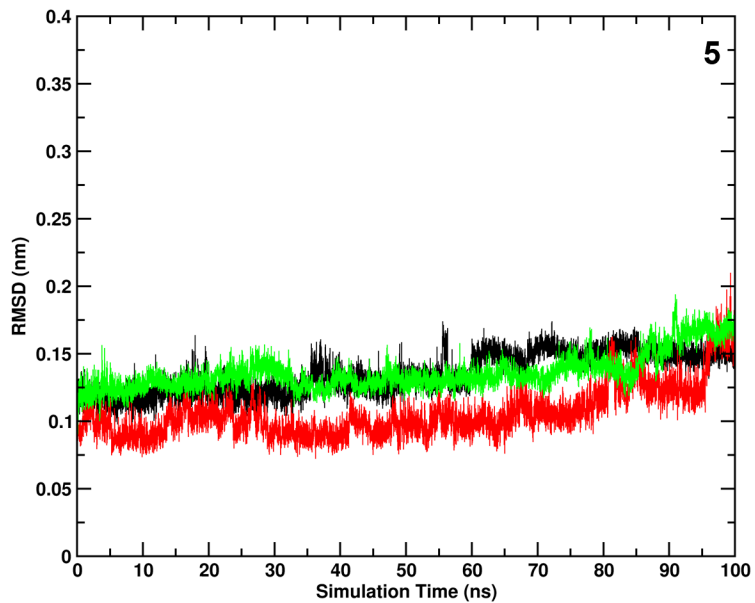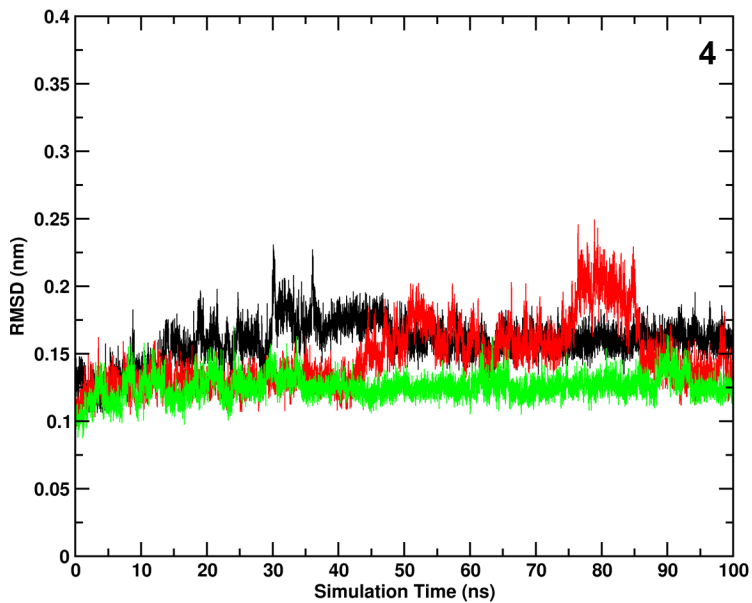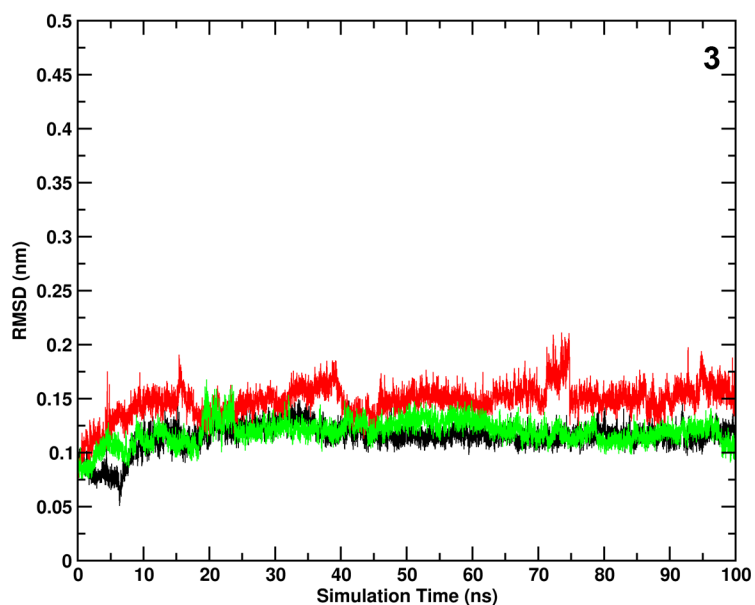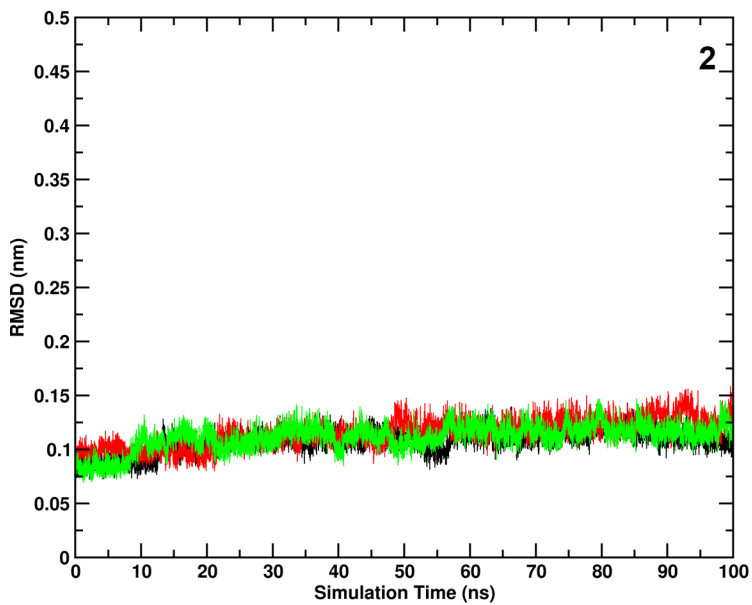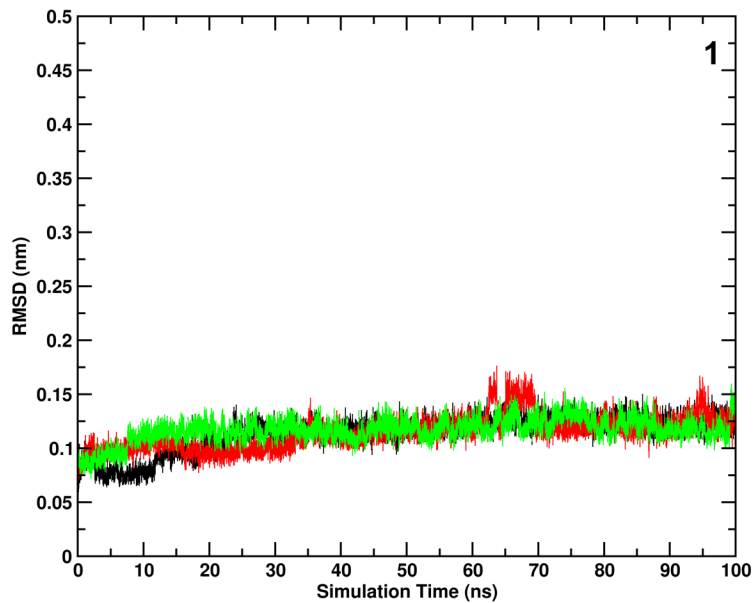common to the triplicate runs.

Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms for N1$_{09}$ Systems

All values relative to post-minimization structre (pre-equilibration)
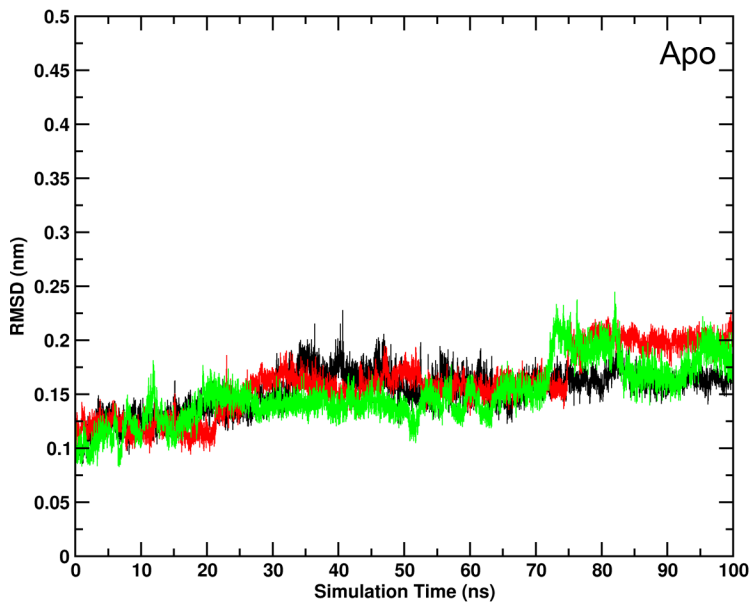common to the triplicate runs.

Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms for N1$_{09}$ Systems

All values relative to post-minimization structre (pre-equilibration)
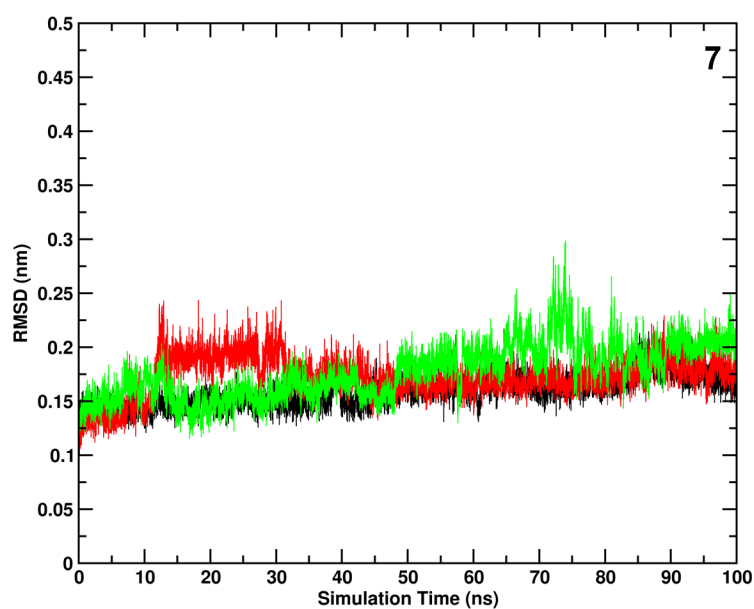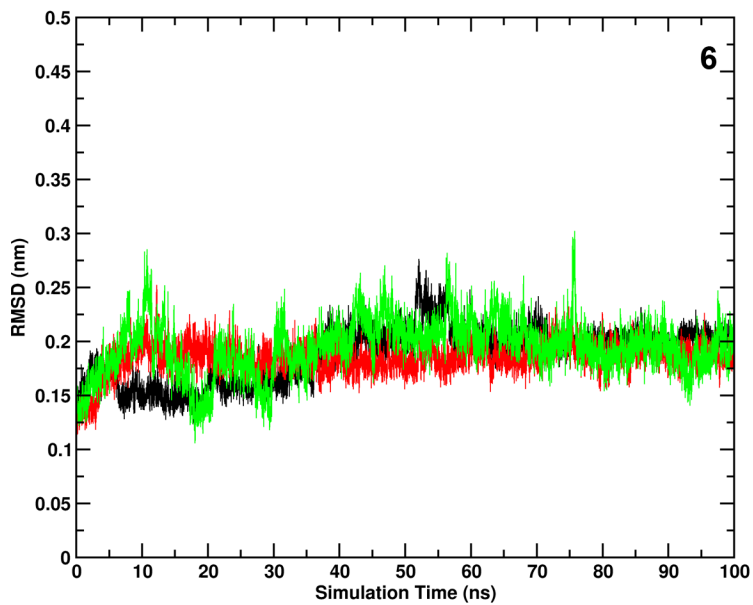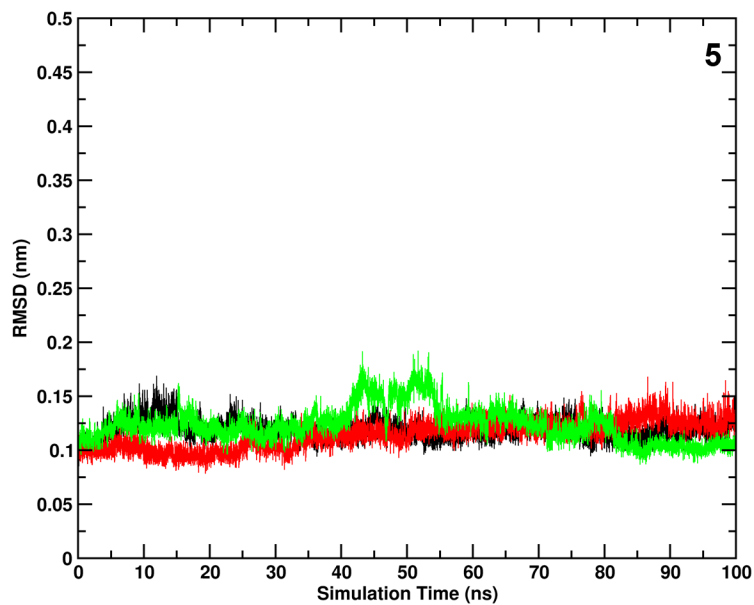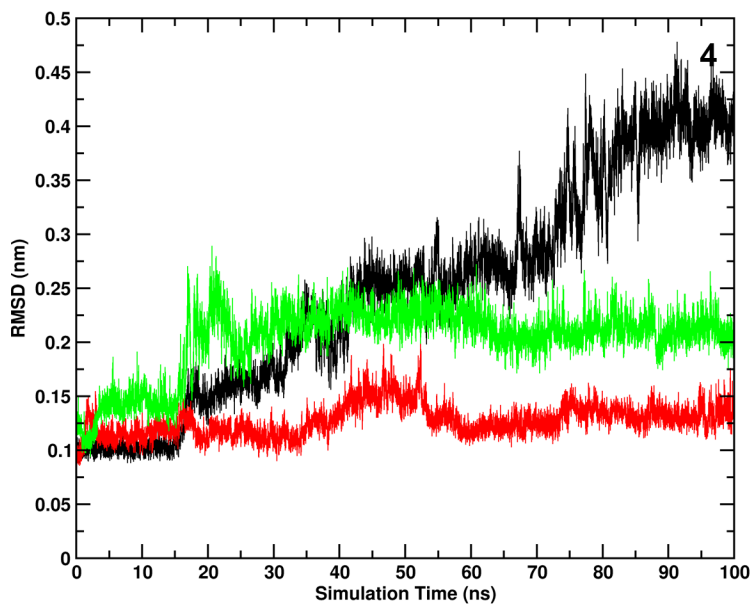common to the triplicate runs.

Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms for N8$_{closed}$ Systems

All values relative to post-minimization structre (pre-equilibration)
common to the triplicate runs.

Root Mean Squared Deviation of Heavy Active Site Atoms for N8closed Systems

All values relative to post-minimization structre (pre-equilibration)
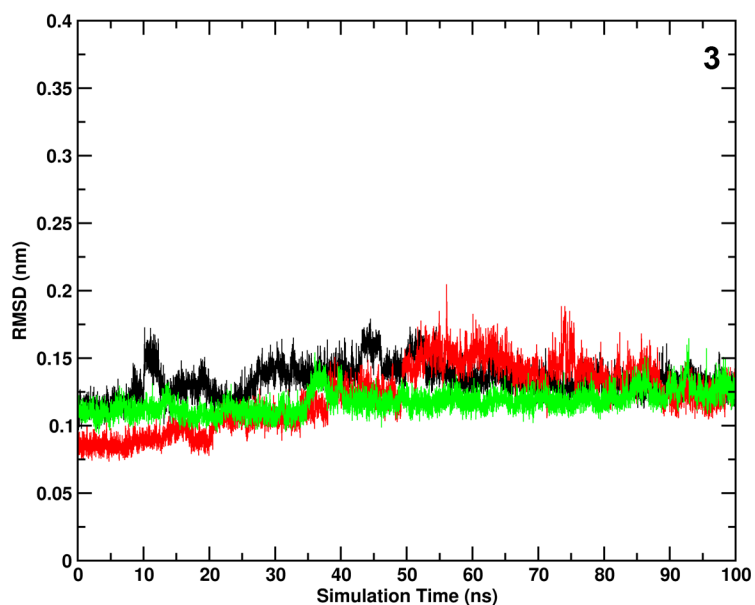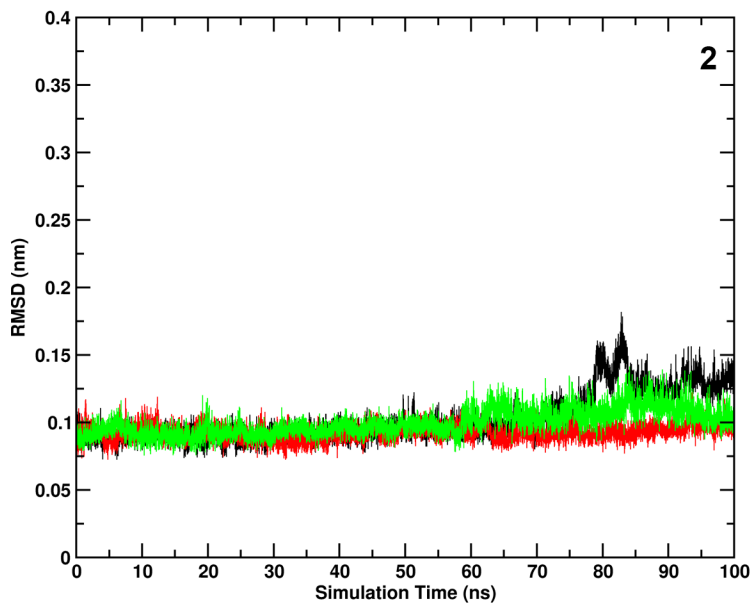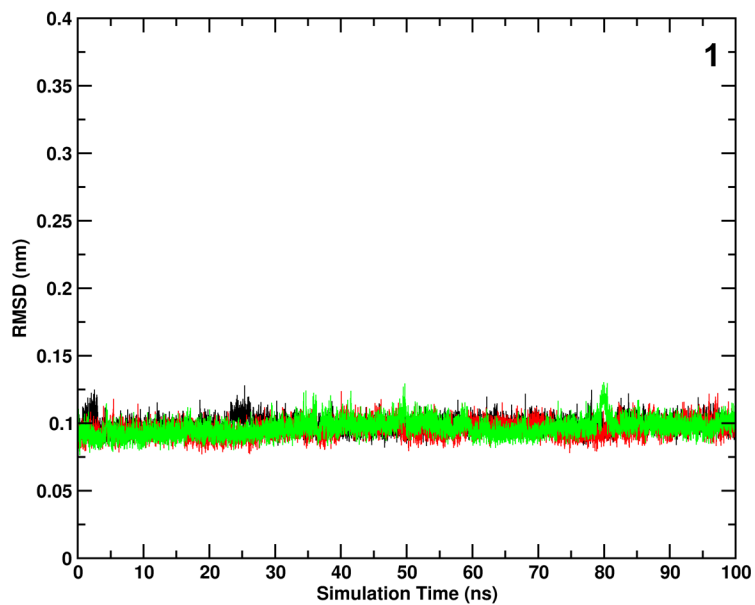common to the triplicate runs.
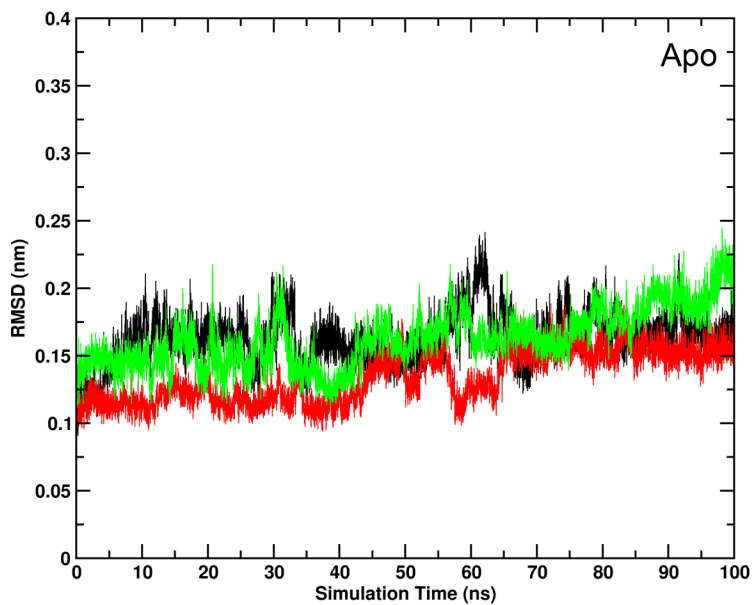
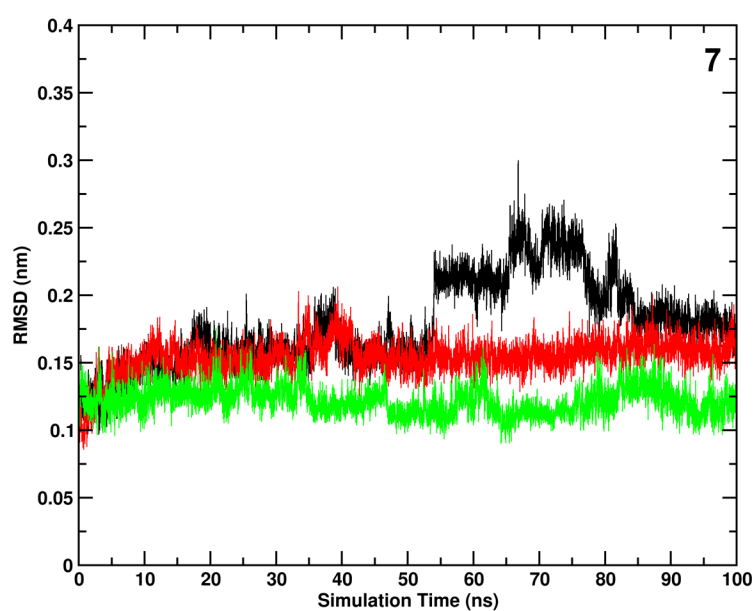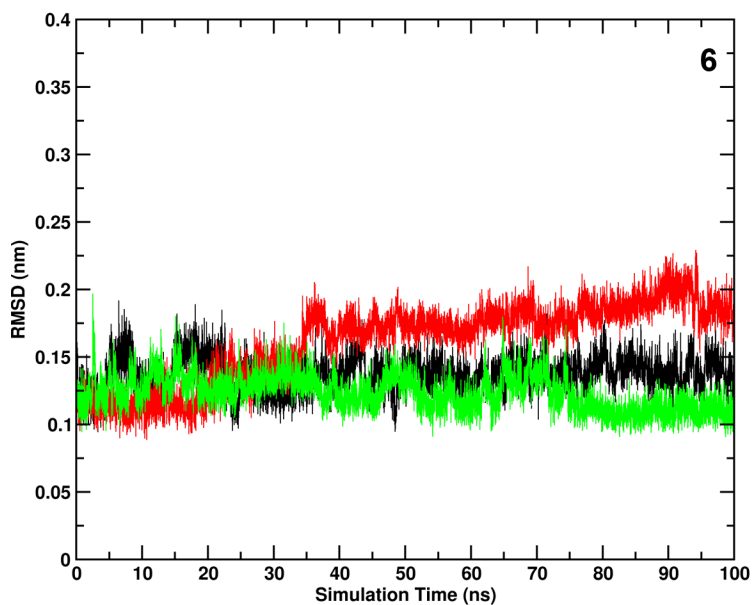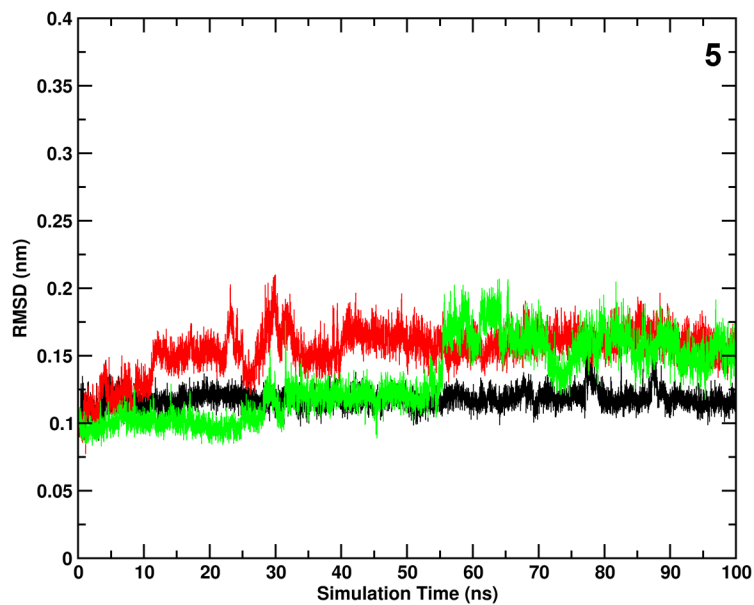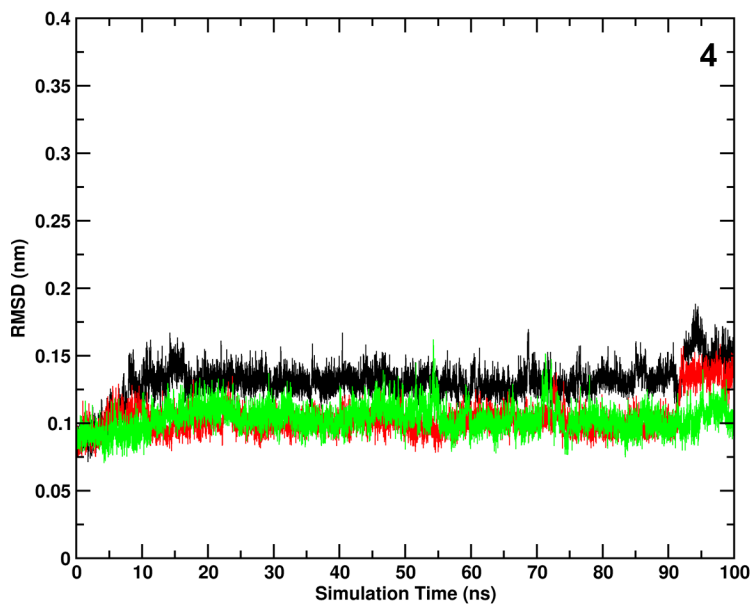# Supporting Information
Text S9

Root Mean Squared Deviation of Heavy Active Site Atoms for N8$_{open}$ Systems

All values relative to post-minimization structre (pre-equilibration)
common to the triplicate runs.

Root Mean Squared Deviation of Heavy Active Site Atoms for N8$_{open}$ Systems

All values relative to post-minimization structre (pre-equilibration)
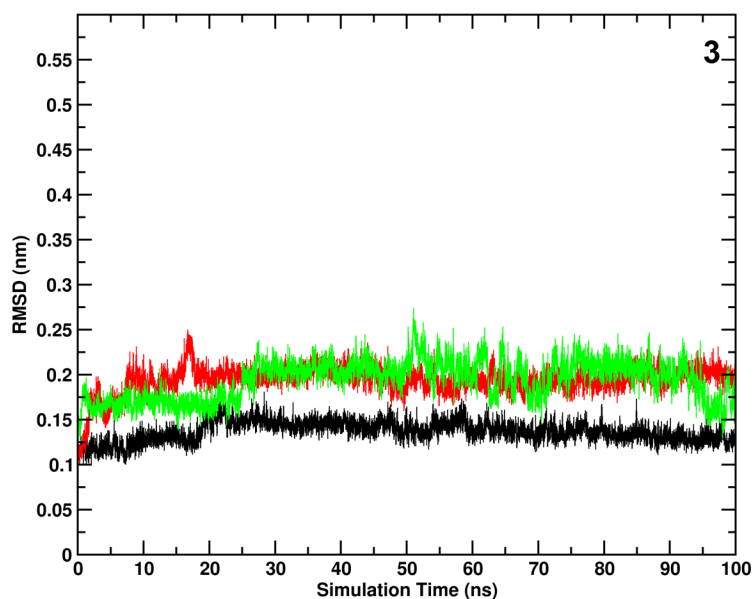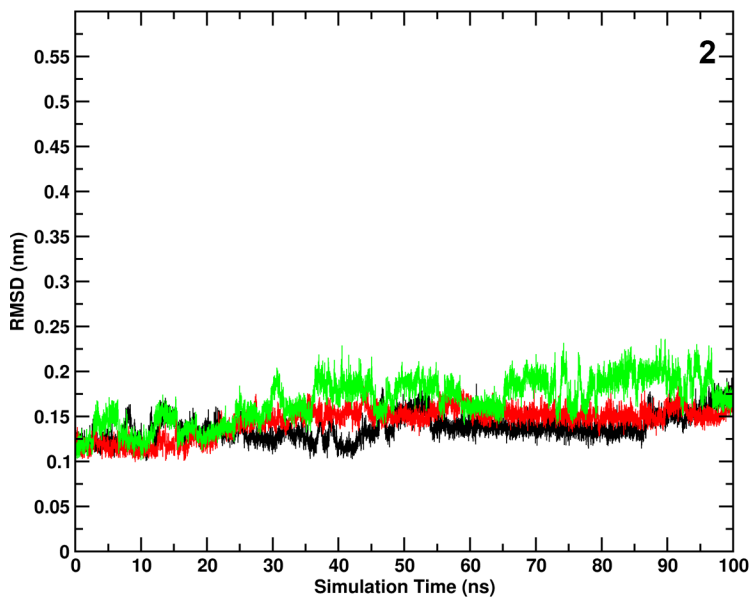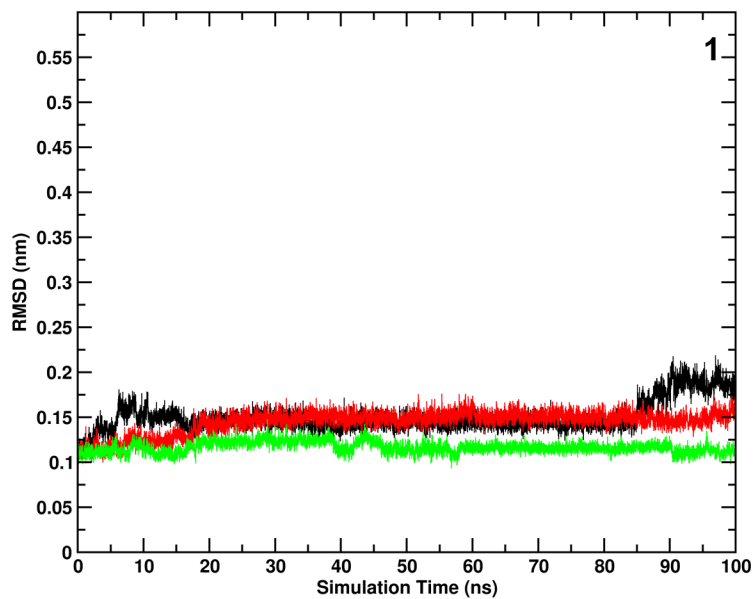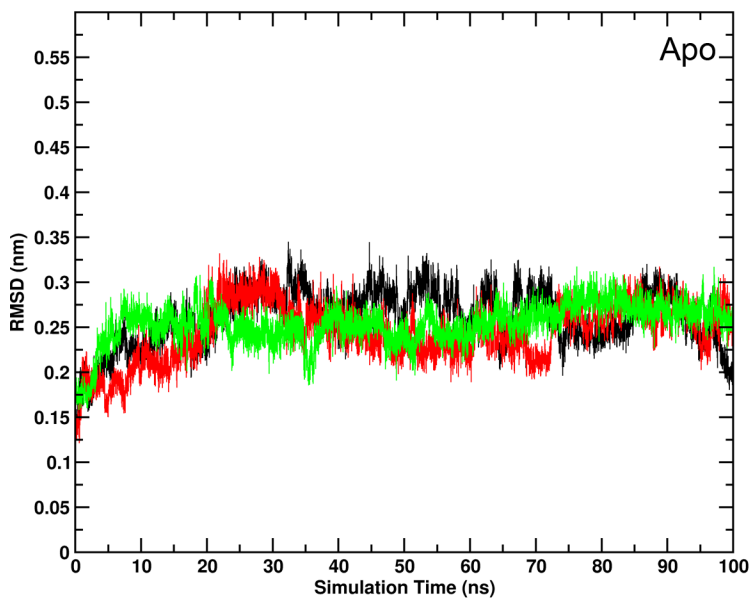common to the triplicate runs.