mucin runs summary

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This is a very brief summary of the mucin runs.

The simulations were run using the pmemd (serial) program in the AMBER suite of molecular modeling tools. They were run in the NPT ensemble at 300 K at 1 atmosphere in explicit TIP3P waters. The FF12SB force field was used for the amino acid residues, and the GLYCAM_06h-1 force field was used for the carbohydrate residues. All runs were minimized, heated to 300 K and then well equilibrated before the production runs from which the trajectories described below were extracted.

The GalNAc runs:

32 runs were begun from 16 NMR starting structures. The two sets of 16 were begun with a different random number seed to ensure sampling of different conformational spaces. 317739 usable frames were extracted from the runs, representing a total of 3.18 microseconds.

The Mannose runs:

36 runs were begun from 35 (*) NMR starting structures. The two runs begun from the same structure were minimized separately, so they sampled different conformational spaces. 355642 usable frames were extracted, representing 3.56 microseconds.

The unglycosylated runs:

48 runs were begun from 47 (*) NMR starting structures. The two runs begun from the same structure were minimized separately, so they sampled different conformational spaces. 520407 usable frames were extracted, representing 5.20 microseconds.

* I'm not sure why, but somehow, in each of these sets, one of the pdb files got used twice, and one got ignored. Everything else appears to be exactly as expected so far.