Video Poster for Mucin Runs

128.192.9.183/eln/lachele/2017/02/23/video-poster-for-mucin-runs

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I need to make videos for the mucin runs, and I can't find most stuff. Also, I need a check-list plan (too much else going on).

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For all videos: Make short trajectories

Make short trajectories, every 200 frames, aligned on name CA and resid 4 5 6 7.

Video Set 1: Mobility compared to NMR structures

- These should have backbone and glycans.
- D suggests doing an end-on video instead or as well. so, try that and end-on

Video Set 2: Backbone Extension Illustration

Video Set: Backbone only, with tube and backbone + heavy atoms for each of the three

- Trying an edgy-glass tube for the first try at this. The video, with smoothing and 1392 frames, takes considerable time, and all 64 G on Rime. With luck it will be done by morning…
- D suggests doing an end-on video instead or as well. so, try that out, too.

Associated Stills 1: Show a single threonine, one with GlcNAc, one with Man and one with just the sidechain (for completeness).

Associated Stills 2:

- Use trajectory with every 200th frame saved
  - I saved the aligned trajectory: GalNAc_bigSet_aligned_THR_back_every-200.mdcrd
  - I saved the VMD visualization state: Back_tube_all_GalNAc.vmd
      I set the tube material (see below) to 'opaque' so that the view doesn't look blank ('glass bubble' hardly shows up on a normal screen).
- Align all THR backbone atoms and save the trajectory
  - In the VMD Trajectory tool, I used "resname OLT and name H N C O CA" to align
  - Instead, use CA C N only
- Get the ~~ribbon~~ for the THR backbone – used "tube" for now. For whatever reason, "new ribbons" and "new cartoon" extend the ribbon past the N-terminus. Weird. But "tube" seems to do what is desired.
  - I set the tube radius to 0.1
  - I tried several materials. Will decide between them later
  - I rendered with tachyon
- Show a reasonable selection from the trajectory all at once, just the ribbons, to give a feel for the range of motion. Make the ribbons a 'glass' material so that the color will be strongest where the most ribbons overlap.
- Do this for all three: protein only, Man, GalNAc
- Save image to go with the video set

Video set 2, maybe:

Might move the single-residue movies Man & GalNAc to the next slide with the phi-psi angles.

Video Set 3: 4-way Bonding Illustration

1. Save a trajectory of only the frames that will be shown.
2. In that trajectory, find a frame with an N-H-O angle around 135-140 and an N-O distance around 3.2. See this post, especially the graph near the top, for the reason.
3. Try getting VMD to do a rock-n-roll on just one frame to learn how it works.
4. Once that works, show all the dots for the O's and H's and make the real one.

Stats slide

Show the Backbone atoms avg rmsd and stdev for all three, also the N-N distance for all three, colored the same, with stills of the

Other things to do

Do a quick 1/r^6 average of the H-H distances.

Write blurb about how/why the multiple runs.