For fitting the molecule to the reference structure for applying orientation restraints, the current structure was shifted by the center of mass of the reference structure instead of the current structure. Obviously, if the molecule doesn't drift much during the simulation, this has little effect. If it moves a lot, the restraining is still correct (unless ensemble averaging is used). The only incorrect output is the orientation of the molecule.

This bug seems to have been present since the first version of the code.

Associated revisions

Revision 74391574 - 08/02/2017 08:27 PM - Berk Hess
Fix orientation restraint reference

The resetting of the COM of the molecule with orientation restraints for fitting to the reference structure was done with the COM of the reference structure instead of the instantaneous structure. This does not affect the restraining (unless ensemble averaging is used), only the printed orientation tensor.

Fixes #2219.

Change-id: l4984ee764780a5c3850feb4bfe4a624afd5cec7

Revision 3e3c2ea0 - 08/03/2017 04:09 PM - Berk Hess
Fix orientation restraint reference

The resetting of the COM of the molecule with orientation restraints for fitting to the reference structure was done with the COM of the reference structure instead of the instantaneous structure. This does not affect the restraining (unless ensemble averaging is used), only the printed orientation tensor.

Fixes #2219.

Change-id: l4984ee764780a5c3850feb4bfe4a624afd5cec7

History

#1 - 07/27/2017 10:13 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2219.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~master~I4984ee764780a5c3850feb4bfe4a624afd5cec7
Gerrit URL: https://gerrit.gromacs.org/6811

#2 - 07/27/2017 10:14 PM - Berk Hess
- Status changed from In Progress to Fix uploaded

#3 - 08/03/2017 11:35 AM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 743915740150ddf5891c213a65405bbda6d3dab4.
Gerrit received a related patchset '1' for Issue #2219.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~I4984ee7f64780a5c3850feb4bfe4a624afd5cec7
Gerrit URL: https://gerrit.gromacs.org/6821

#5 - 08/03/2017 03:05 PM - Mark Abraham
- Target version changed from 2018 to 2016.4

#6 - 08/03/2017 03:06 PM - Mark Abraham
- Status changed from Resolved to Closed