Wrong improper dihedral for HYP

From gromos4x to gromos5x the improper dihedral of Hydroxyproline was changed, which produces the wrong isomer. There is no indication for this in the publication by Oostenbrink et. al. [1].

I propose the following fix: https://gerrit.gromacs.org/#/c/6675/

[1] JCC 2004 vol 25 pag 1656

History

#1 - 05/31/2017 03:29 PM - Gerrit Code Review Bot
Gerrit received a related patchset '3' for Issue #2195.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~I0a85b3eeea1c57759925f6206e574b7e3ce847aa
Gerrit URL: https://gerrit.gromacs.org/6675

#2 - 05/31/2017 08:38 PM - Szilárd Páll
- Status changed from New to In Progress

#3 - 06/02/2017 01:00 PM - Berk Hess
The description is too concise to understand.
I understand that order has changed from GROMOS release 4x to 5x.
But does 4x or 5x give the wrong isomer?
Our GROMOS force field files have been automatically converted from original GROMOS files, so those should match an old GROMOS version, but I don't know if that would be 4x.
I can ask Alessandra.

#4 - 06/02/2017 06:25 PM - Mark Abraham
Berk Hess wrote:

> The description is too concise to understand.
> I understand that order has changed from GROMOS release 4x to 5x.
> But does 4x or 5x give the wrong isomer?
> Our GROMOS force field files have been automatically converted from original GROMOS files, so those should match an old GROMOS version, but I don't know if that would be 4x.
> I can ask Alessandra.

There was discussion on the gerrit patch and Philip has emailed the GROMOS contact address to follow up (which I have forwarded to Berk)

#5 - 09/12/2017 11:46 AM - Mark Abraham
- Target version changed from 2016.4 to 2016.5

From memory, the email discussion concluded that there was an issue in the way GROMOS implemented the approach, but it was not yet clear whether there was an issue GROMACS should address.

#6 - 01/03/2018 06:23 PM - Mark Abraham
- Status changed from In Progress to Rejected

04/04/2020
If someone knows what/if we should change, do let us know. Rejecting until we know we have a problem.