GROMACS - Bug #1276

pdb2gmx ignores angles when no bonds are present

06/05/2013 06:03 PM - Justin Lemkul

Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: preprocessing (pdb2gmx,grompp)
Target version: 5.0
Affected version - extra info: Difficulty: uncategorized
Affected version: 4.6

Description
As recently posted on gmx-users, pdb2gmx will not write angles if bonds do not connect the constituent atoms, despite being present in an .rtp [angles] directive. For most purposes, this is not a problem, but there are specialty force fields that need such behavior. I have attached a much simpler test case than the original gmx-users post to reproduce the problem. Invoke with:

echo 1 3 | pdb2gmx -f water.pdb

Related issues:
Related to GROMACS - Bug #1711: gmx x2top seg fault

Associated revisions
Revision 7ba0a841 - 06/29/2014 08:04 AM - Erik Lindahl
Enable rtp angle/dihedral entries not connected by bonds

pdb2gmx has previously silently ignored any angles or torsions not connected by bonds. This patch adds code to mark with RTP/hackblock entries that have been assigned in this search, and afterwards we add those that have not yet been matched. In particular, this makes it possible to have angles or torsions in RTP entries even if those atoms are not connected by bonds.

Fixes #1276.

Change-Id: I61c3c3954ef8c4cd59956d88b73c6a69c1a66c65

History
#1 - 06/05/2013 08:08 PM - David van der Spoel
- Tracker changed from Bug to Feature

pdb2gmx is for biomolecules only. Acypype and friends can be used for GAFF etc.

#2 - 06/05/2013 08:12 PM - Justin Lemkul
I agree that there are plenty of ways outside of pdb2gmx that can generate topologies, but when pdb2gmx silently ignores an otherwise properly formatted .rtp entry, I think there’s still a problem worth fixing. Nowhere in the documentation does it say that pdb2gmx can only be used for biomolecules, it says that it reads a list of input files and writes a topology. If we need to be more specific about limitations, that’s fine, but when input files are written correctly (with respect to what the manual says), the end user is going to assume that the outcome will be correct, but in this case, it is not.

#3 - 06/22/2014 10:18 PM - Erik Lindahl
- Tracker changed from Feature to Bug
- Affected version set to 4.6

Agree with Justin that this is a bug - either in the implementation or documentation.

#4 - 06/24/2014 03:54 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1276.
I'm not sure how to fix the implementation, but I added a note to the documentation for now.

Uploader: Erik Lindahl (erik@kth.se)
Change-id: I61c3c3954ef8c4cd59956d88b73c6a69c1a66c65
Gerrit URL: https://gerrit.gromacs.org/3686

- Status changed from New to Fix uploaded
- Status changed from Fix uploaded to Closed
- Assignee changed from David van der Spoel to Erik Lindahl
- Target version changed from future to 5.0

Related to Bug #1711: gmx x2top seg fault added

Files

| files.tgz | 61.5 KB | 06/05/2013 | Justin Lemkul |