

GROMACS - Bug #2577

pdb2gmx chainsep is broken

07/18/2018 10:58 AM - Joe Jordan

Status:	Closed	Difficulty:	uncategorized
Priority:	High		
Assignee:	Joe Jordan		
Category:	preprocessing (pdb2gmx,grompp)		
Target version:	2019		
Affected version - extra info:			
Affected version:	git master		

Description

In the course of developing tests for pdb2gmx -chainsep flag, I realized that this flag is currently broken. The tarballs for 2018.1 and 2018.2 are not affected.

After performing git bisect, the first bad commit is "Remove mols from gmx_mtop_t"
[8dd3c9ae88004054b3b112c23f747d27a19d8d29](https://github.com/gromacs/gromacs/commit/8dd3c9ae88004054b3b112c23f747d27a19d8d29)

Associated revisions

Revision 4ad3d382 - 08/22/2018 01:34 PM - Joe Jordan

Fix pdb2gmx -chainsep

Fixes #2577

This patch makes readConfAndAtoms public and has pdb2gmx call it directly. Previously pdb2gmx called readConfAndTopology, which then called readConfAndAtoms and then tpx_make_chain_identifiers, the latter of which is suspected of being broken, as documented in the TODO added here.

Change-Id: I1b47e1743f6accf77ae67d232eb2c815edcff970

History

#1 - 07/18/2018 02:14 PM - Mark Abraham

- Description updated

#2 - 07/18/2018 03:39 PM - Mark Abraham

- Target version changed from 2018.3 to 2019

- Affected version changed from 2018.3 to git master

If I understand Joe correctly, that commit is on master branch, so 2018.x is demonstrably unaffected

#3 - 07/18/2018 05:45 PM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue [#2577](#).

Uploader: Joe Jordan (e.jordan12@gmail.com)

Change-Id: gromacs~master~I41a215b53e3a4bace7738c838f426047e6937d57

Gerrit URL: <https://gerrit.gromacs.org/8089>

#4 - 07/19/2018 12:49 PM - Joe Jordan

The issue turned out to be that fillMoleculeIndices increments globalMolIndex (which becomes top.mols) at the beginning rather than the end of the for loop.

#5 - 08/07/2018 03:22 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2577](#).

Uploader: Joe Jordan (e.jordan12@gmail.com)

Change-Id: gromacs~master~I1b47e1743f6accf77ae67d232eb2c815edcff970

Gerrit URL: <https://gerrit.gromacs.org/8147>

#6 - 08/08/2018 08:40 PM - Joe Jordan

Further testing has shown that <http://redmine.gromacs.org/projects/gromacs/repository/revisions/8dd3c9ae88004054b3b112c23f747d27a19d8d29> does cause a change in behavior. Both before and after the change pdb file reading works correctly and the chainnum and chainid are read in correctly by readConfAndTopology in confio.cpp when this function is called by read_tps_conf in the same file. The function read_tps_conf is called directly by the pdb2gmx function read_pdball. Everything is the same up to when gmx_mtop_t_to_t_topology is called a few lines below readConfAndTopology. In this function, using as input a pdb file with only protein (I tried one and multiple chains and the results are the same) top.mols gets set as 0 before the change in question and as 1 after.

#7 - 08/22/2018 02:00 PM - Joe Jordan

- Status changed from New to Resolved

Applied in changeset [4ad3d382ad4e45961e1105254208f6e54008deeb](#).

#8 - 09/10/2018 02:24 PM - Paul Bauer

- Status changed from Resolved to Closed