GROMACS - Bug #2370

pdb2gmx does not report why chains of residues are terminated

01/02/2018 08:16 AM - Mark Abraham

Status: Closed
Priority: Normal
Assignee:
Category:
Target version:
Affected version - extra info: affects all versions
Affected version: 2016.5
Difficulty: uncategorized

Description

In `find_nc_ter()`, the chain is terminated when a residue is found whose type does not match that of the rest of the chain. This happens frequently when users modify a residue and forget to change `residuetypes.dat`.

We should at least report the reason for the termination, so the user being prompted for a C terminus after the residue before the modified one can see why they are being prompted. Perhaps we should also suggest editing `residuetypes.dat` when this occurs.

Associated revisions

Revision 541e7d05 - 01/10/2018 10:51 AM - Erik Lindahl

Improve pdb2gmx for nonstandard residue types

If explicit non-blank chain identifiers are set, it will now be a hard error if the residue types in each chain do not match. For blank chain ID we still need to allow detection of non-chain parts, but this case too now provides more explicit output information.

Fixes #2370.

Change-id: lc70f4d91fddd80a22e91eb1a0672a15838966a75

History

#1 - 01/02/2018 11:56 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2370.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-id: gromacs~release-2018~lc70f4d91fddd80a22e91eb1a0672a15838966a75
Gerrit URL: https://gerrit.gromacs.org/7412

#2 - 01/02/2018 01:26 PM - Erik Lindahl

- Status changed from New to Fix uploaded

#3 - 01/10/2018 12:39 PM - Erik Lindahl

- Status changed from Fix uploaded to Resolved

Applied in changeset 541e7d05da570755b263f5ada97215b96e61781c.

#4 - 02/28/2018 11:27 PM - Erik Lindahl

- Status changed from Resolved to Closed