

GROMACS - Bug #2028

hdb file can't handle empty lines

08/09/2016 07:12 AM - Chris Neale

Status: Closed	
Priority: Low	
Assignee: Erik Lindahl	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 2018	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.1.2	

Description

When the .hdb file has empty lines, it does not seem to be read in properly by pdb2gmx.

test:

A. Use opslaa.ff

B. modify aminoacids.hdb by adding an empty line as the very first line (other places with empty lines in this file also cause things not to be read below the empty line, but I do not show that here).

RESULT of pdb2gmx -ter -ignh:

Checking for duplicate atoms....

Generating any missing hydrogen atoms and/or adding termini.

Now there are 3 residues with 28 atoms

Making bonds...

WARNING: atom HA is missing in residue MET 1 in the pdb file

You might need to add atom HA to the hydrogen database of building block MET in the file aminoacids.hdb (see the manual)

WARNING: atom HB1 is missing in residue MET 1 in the pdb file

You might need to add atom HB1 to the hydrogen database of building block MET in the file aminoacids.hdb (see the manual)

WARNING: atom HB2 is missing in residue MET 1 in the pdb file

You might need to add atom HB2 to the hydrogen database of building block MET in the file aminoacids.hdb (see the manual)

... (there are many more like this)

But it works just fine with the standard .hdb file.

There is an obvious workaround for this. I ran into it when adding a blank line before a comment (after having been scared away from even trying to create multiple .hdb files based on issues 2026 and 2027 but still wanting to note my modification in the .hdb file). Note that comments beginning with semicolons do seem to be handled correctly in the .hdb file and even a line with a space and then the semi-colon does not break .hdb parsing.

There is no good reason to desire blank lines in the .hdb file, just that a user might add one thinking it was OK, since many other force field file types can handle it. If there is a desire not to allow blank lines in the .hdb file, then perhaps throwing an error is better than simply not finding the hydrogens.

Associated revisions

Revision 3993194e - 01/02/2018 09:10 PM - Erik Lindahl

Allow empty lines in hdb files

Skip lines that consist only of whitespace. Not a universal solution for fixing hdb files, but better than the user getting very strange error messages that don't say anything about whitespace.

Fixes #2028.

Change-Id: I0962c89d0251f83da7fe0440efd31fb7ca468690

History

#1 - 08/09/2016 07:34 AM - Chris Neale

possibly related to this: http://gromacs.org_gmx-users.maillist.sys.kth.narkive.com/Bm5x5aOa/problem-in-hdb-file

#2 - 12/31/2017 02:23 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2028](#).

Uploader: Erik Lindahl (erik.lindahl@gmail.com)

Change-Id: gromacs~release-2018~l0962c89d0251f83da7fe0440efd31fb7ca468690

Gerrit URL: <https://gerrit.gromacs.org/7405>

#3 - 12/31/2017 02:24 PM - Erik Lindahl

- Status changed from New to Fix uploaded

#4 - 12/31/2017 03:06 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2028](#).

Uploader: Erik Lindahl (erik.lindahl@gmail.com)

Change-Id: gromacs~release-2018~le7bf8e65892281cc2744146a5525be0c4afdcecf

Gerrit URL: <https://gerrit.gromacs.org/7406>

#5 - 01/01/2018 10:56 AM - Mark Abraham

- Category set to preprocessing (pdb2gmx.grompp)

- Assignee set to Erik Lindahl

- Target version set to 2018

#6 - 01/02/2018 09:10 PM - Erik Lindahl

- Status changed from Fix uploaded to Resolved

#7 - 01/02/2018 09:11 PM - Erik Lindahl

- Status changed from Resolved to Closed