GROMACS - Feature #720

permit pdb2gmx to choose a kind of HIS based on proton position

03/13/2011 02:09 PM - David van der Spoel

Status:	Accepted	
Priority:	Low	
Assignee:		
Category:	preprocessing (pdb2gmx,grompp)	
Target version:	future	
Difficulty:	simple	

Description

In release-4-5-patches and most likely all other pdb2gmx variants the hydrogens are ignored for selecting the HIS type.
The attached peptide may be used for testing:
pdb2gmx -f hid.pdb -ff amber99sb -water tip3p
will crash due to non-existence of HE2 while HD1 is present.

History

#1 - 06/08/2011 03:53 PM - Rossen Apostolov

- Target version changed from 4.5.4 to 4.5.5

#2 - 09/22/2011 03:45 PM - Rossen Apostolov

- Target version changed from 4.5.5 to 4.5.6

#3 - 03/05/2012 11:21 AM - Berk Hess

- Status changed from New to Feedback wanted

With 4.5.5 I get:
Fatal error:
Atom HD1 in residue HIS 23 was not found in rtp entry HIE with 17 atoms
while sorting atoms.

This is a correct error message right?

Could you check again with 4.5.5?

#4 - 03/05/2012 11:50 AM - David van der Spoel

Just recompiled the release-4-5-patches tree and error is still there.

#5 - 04/11/2012 10:15 AM - Rossen Apostolov

- Priority changed from Normal to High

#6 - 04/12/2012 09:31 PM - Rossen Apostolov

With the latest 4-5-patches:

@Program pdb2gmx, VERSION 4.5.5-dev-20120411-66c78
Source code file: /home/rossen/Gromacs-dev/gromacs/src/kernel/pdb2gmx.c, line: 655

Fatal error:
Atom HD1 in residue HIS 23 was not found in rtp entry HIE with 17 atoms
while sorting atoms.
@

So we can close it, right?

#7 - 04/12/2012 10:35 PM - David van der Spoel

Nope. For this peptide pdb2gmx should decide that it is a HID residue, not a HIE. If you add -ignh it can do what it likes. For structures from NMR that need to be pdb2gmx-ed while keeping the hydrogens this will cause serious problems. 10% of the HIS residues are HID in solution, in proteins I don't know the statistics.

#8 - 04/16/2012 11:52 AM - Berk Hess

- Category set to preprocessing (pdb2gmx,grompp)

- Priority changed from High to Normal

- Target version changed from 4.5.6 to 4.6

It seems that this issue is now more of a feature request than a real bug. pdb2gmx decided the protonation state of His based on the environment, not based on the actual protons, if they are present. The pdb file can be processed as you want using pdb2gmx -his
It would be nice to decide state based on the actual protons, but this is not a very common case. So someone interested in this should add this feature.

#9 - 04/16/2012 11:52 AM - Rossen Apostolov

- Tracker changed from Bug to Feature

#10 - 12/28/2012 11:59 PM - Erik Lindahl

- Priority changed from Normal to Low

- Target version changed from 4.6 to 5.0

Nice feature to have at some point, but not for 4.6. As Berk commented, that functionality is already possible by using the "-his" flag. Changing target to 5.0.

#11 - 01/09/2014 01:56 PM - Rossen Apostolov

- Target version changed from 5.0 to 5.x

this won't be in 5.0. Keeping it open in case someone is interested in implementing it eventually.

#12 - 10/14/2015 06:18 PM - Mark Abraham

- Target version changed from 5.x to future

#13 - 11/17/2016 03:51 PM - Mark Abraham

- Subject changed from pdb2gmx ignores hydrogens when selecting HIS to permit pdb2gmx to choose a kind of HIS based on proton position

- Status changed from Feedback wanted to Accepted

- Assignee deleted (David van der Spoel)

- Difficulty simple added

- Difficulty deleted (uncategorized)

Updated to reflect status

Files

hid.pdb	2.88 KB	03/13/2011	David van der Spoel