

GROMACS - Bug #1133

Charmm27 HIS Heme Bond pdb2gmx 'HIS1' error

01/27/2013 02:45 AM - Grant Rotskoff

Status: Closed	
Priority: Low	
Assignee: Berk Hess	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 5.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 4.6	
Description	
When a HIS / Heme bond is detected by pdb2gmx in the Charmm27 ff, it fails to convert the 'HIS1' residue to 'HSD'. This is fixed by adding HIS1 HSD to aminoacids.r2b	

Associated revisions

Revision 84d76486 - 06/12/2014 12:05 AM - Rossen Apostolov

Mapped HIS1 to HSD in charmm27.

Fixes #1133.

Change-Id: I6c289af9b58c8e7cd66f36982bf118505aa38f7d

History

#1 - 05/26/2014 03:52 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1133](#).

Uploader: Rossen Apostolov (rossen@kth.se)

Change-Id: I6c289af9b58c8e7cd66f36982bf118505aa38f7d

Gerrit URL: <https://gerrit.gromacs.org/3511>

#2 - 05/26/2014 03:53 PM - Rossen Apostolov

- Status changed from New to Fix uploaded

- Target version set to 5.0

- Affected version set to 4.6

#3 - 06/12/2014 12:05 AM - Erik Lindahl

- Status changed from Fix uploaded to Resolved

#4 - 06/12/2014 12:05 AM - Erik Lindahl

- Status changed from Resolved to Closed