### Gromacs - Bug #1133

**Charmm27 HIS Heme Bond pdb2gmx 'HIS1' error**

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Affected version: 4.6</td>
</tr>
</tbody>
</table>

**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: l6c289af9b58c8e7cd66f36982bf118505aa38f7d

**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: l6c289af9b58c8e7cd66f36982bf118505aa38f7d

Gerrit URL: [https://gerrit.gromacs.org/3511](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