GROMACS - Feature #2272

pdb2gmx does not accept tips3p as a water model

10/13/2017 06:30 PM - David van der Spoel

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td></td>
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<tr>
<td>Target version:</td>
<td>2018</td>
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<tr>
<td>Difficulty:</td>
<td>simple</td>
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**Description**

Despite being supported by gromacs, pdb2gmx does not accept tips3p as a water model. This should be fixed since it is the default water model in charm. 

**Associated revisions**

Revision 6d6a726e - 10/30/2017 02:26 PM - David van der Spoel

Added option -water tips3p to pdb2gmx.

Fixes #2272

Change-Id: lbfc63009767fd667df51ff10041791268351e1ca

**History**

#1 - 10/13/2017 06:37 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2272.

Uploader: David van der Spoel (davidvanderspoel@gmail.com)

Change-Id: gromacs~master~Ibfc63009767fd667df51ff10041791268351e1ca

Gerrit URL: https://gerrit.gromacs.org/7039

#2 - 10/30/2017 02:26 PM - Mark Abraham

- Target version set to 2018

#3 - 10/30/2017 02:51 PM - David van der Spoel

- Status changed from Accepted to Resolved

Applied in changeset 6d6a726eb453579a34b4761240c8029ff5aade.

#4 - 11/28/2017 05:59 PM - Mark Abraham

- Status changed from Resolved to Closed