

## GROMACS - Feature #2272

### pdb2gmx does not accept tips3p as a water model

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

|  |                     |
|--|---------------------|
| <b>Status:</b>   | Closed              |
| <b>Priority:</b>   | Low                 |
| <b>Assignee:</b>   | David van der Spoel |
| <b>Category:</b>   |                     |
| <b>Target version:</b>   | 2018                |
| <b>Difficulty:</b>   | simple              |
| <b>Description</b>   |                     |
| 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 charmm. |                     |

#### 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](mailto:davidvanderspoel@gmail.com))

Change-Id: gromacs~master~lbfc63009767fd667df51ff10041791268351e1ca

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 [6d6a726eb453573a34b476f1240c8029ff5aade](#).

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

- Status changed from Resolved to Closed