gmx wham uses conversion from kJ to kcal inconsistent with the rest of GROMACS

10/08/2015 07:31 PM - James Barnett

Status: Closed
Priority: Normal
Assignee: James Barnett
Category: Target version:
Affected version - extra info:
Affected version: git master

Difficulty: uncategorized

Description

Associated revisions
Revision a1c6f9be - 10/12/2015 02:32 PM - James Barnett


Also fixes #1841.

Change-Id: Id810fe0c0df82e0f9a05c294144a036534d4856c

History
#1 - 10/08/2015 07:36 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1841.
Uploader: James "Wes" Barnett (jbarnet4@tulane.edu)
Change-Id: ld810fe0c0df82e0f9a05c294144a036534d4856c
Gerrit URL: https://gerrit.gromacs.org/5191

#2 - 10/08/2015 08:55 PM - James Barnett

I can't edit the title but I should say that the value in gmx wham is different from the one used in the rest of the project's code, so it's only "wrong" in that sense (international vs. thermochemical definitions).

#3 - 10/12/2015 12:44 PM - Mark Abraham

- Subject changed from gmx wham uses wrong conversion from kJ to kcal to gmx wham uses conversion from kJ to kcal inconsistent with the rest of GROMACS

#4 - 10/12/2015 02:45 PM - James Barnett

- Status changed from New to Resolved

Applied in changeset a1c6f9beb3ff7b2d2227737047148ba4687dea08.

#5 - 10/13/2015 09:42 AM - David van der Spoel

- Status changed from Resolved to Closed