GROMACS - Feature #1564

g_gyrate help text and manual is confusing

07/16/2014 10:40 AM - David van der Spoel

Status: Closed
Priority: Low
Assignee: David van der Spoel
Category: 
Target version: 5.0.7
Difficulty: uncategorized

Description
A clearer specification of the meaning of the components of the radius of gyration should be added. Right now it is not obvious that
\[ R_g(x) = \sqrt{\frac{\sum_i m_i (R_i(y)^2 + R_i(z)^2)}{\sum_i m_i}}. \]

Associated revisions
Revision bc90186c - 06/20/2015 08:10 PM - Erik Lindahl
Updated docs for g_gyrate
Added the equations we use for the axis components.
Fixes #1564.
Change-Id: Ifce17326f738a72386bf24f949e418d2550568b5

History
#1 - 09/01/2014 03:03 PM - Mark Abraham
- Target version changed from 5.0.1 to 5.x

#2 - 06/19/2015 10:04 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1564.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: Ifce17326f738a72386bf24f949e418d2550568b5
Gerrit URL: https://gerrit.gromacs.org/4746

#3 - 06/19/2015 10:04 AM - Erik Lindahl
- Status changed from New to Fix uploaded

#4 - 06/22/2015 12:42 PM - Rossen Apostolov
- Status changed from Fix uploaded to Closed

#5 - 07/11/2016 07:47 PM - Mark Abraham
- Target version changed from 5.x to 5.0.7