

GROMACS - Feature #895

g_rmsf previous frame as reference

03/08/2012 05:47 PM - Manuel Luitz

Status:	In Progress
Priority:	Normal
Assignee:	
Category:	
Target version:	future
Difficulty:	uncategorized
Description	
<p>The previous frame of a trajectory can be used as reference structure instead of the fixed frame given with the -s flag. With this measure, the relative mobility of an atom during the simulation can be measured.</p> <p>The patch invents a new commandline switch -prev to the g_rmsf tool.</p> <p>This patch includes the fix for Bug #894</p>	

History

#1 - 08/04/2012 11:38 PM - Roland Schulz

Could you please upload the patch to gerrit.gromacs.org? Please let us know on gmx-developers@gromacs.org if you have any problems.

#2 - 01/15/2013 07:15 PM - Mark Abraham

- Target version set to future

<https://gerrit.gromacs.org/#/c/1462/> needs to go on master branch

#3 - 04/29/2013 07:39 PM - Mark Abraham

- Status changed from New to Accepted

#4 - 04/29/2013 07:39 PM - Mark Abraham

- Status changed from Accepted to In Progress

<https://gerrit.gromacs.org/#/c/2137/>

Files

g_rmsf-correct-rmsdev_prev-feature.patch	2.39 KB	03/08/2012	Manuel Luitz
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