

GROMACS - Feature #1247

fix hardcoded references to atom names in analysis tools

05/10/2013 02:20 PM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:	Mark Abraham	
Category:	analysis tools	
Target version:	future	
Difficulty:	uncategorized	
Description		
Analysis tools tend to have code that is based on assumptions about atom names, that (e.g.) get invalidated when we add CHARMM into the mix, because it names amide nitrogen HN, not H. Several past bug-fixes have fixed individual cases of this.		
This kind of stuff should be re-implemented, either by calling the selection machinery with logic that is constructed in a single place, or by deprecating a specific tool in favour of calling a general tool with a specific selection.		
Related issues:		
Related to GROMACS - Bug #953: fix for g_chi omega angle calculation	Closed	06/02/2012

History

#1 - 05/10/2013 02:21 PM - Mark Abraham

- Description updated

#2 - 05/22/2013 05:36 AM - Mark Abraham

- Target version changed from future to 5.0

#3 - 05/22/2013 05:36 AM - Mark Abraham

- Assignee changed from David van der Spoel to Mark Abraham

#4 - 05/13/2014 09:33 AM - Mark Abraham

- Target version changed from 5.0 to future

#5 - 06/12/2014 01:20 AM - Erik Lindahl

- Tracker changed from Bug to Feature

One could argue that the present behavior is buggy, but since it was intentionally (=stupidly) coded this way, I'm changing it to a feature since we'll need to rework things quite a bit.