GROMACS - Bug #1235

peptide dihedral angle definitions violate IUPAC

04/30/2013 01:37 AM - Mark Abraham

Status:	New		
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	future		
Affected version - extra info:	probably all versions since prehistoric times	**Difficulty:**	uncategorized
Affected version:	4.6.1		

Description

(and related code probably does who knows what other nasty stuff!)

Standard IUPAC definititions of phi/psi/omega angles (http://www.chem.qmul.ac.uk/iupac/misc/ppep3.html#320) are only vaguely followed by the code for g_chi. Perhaps other code like g_rama or g_angle has related problems.

These definitions should follow IUPAC and probably be implemented via selections in 5.0. At the very least, the lookups via atom names should be consolidated in one place. Numerous bugs have already been revealed by the CHARMM convention of naming hydrogen bonded to nitrogen as "NH", which was not anticipated by the original developers of various GROMACS tools, who hard-coded other strings in multiple places.

Related issues:

Related to GROMACS - Bug #953: fix for g_chi omega angle calculation	**Closed**	**06/02/2012**
Related to GROMACS - Bug #1481: g_chi output file chi.log reports atomic defi...	**New**	**04/11/2014**

History

#1 - 06/18/2014 03:43 PM - Rossen Apostolov

- Related to Bug #1481: g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files added

#2 - 06/19/2014 11:19 PM - Erik Lindahl

- Target version changed from 5.0 to 5.x

#3 - 06/19/2015 12:24 AM - Erik Lindahl

- Target version changed from 5.x to future