Gromacs - Bug #896
CHARMM atom naming in g_helix
03/08/2012 11:27 PM - Justin Lemkul

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: analysis tools
Target version: 4.5.6
Affected version - extra info: 4.5.5

Description
Similar to bug #788, the naming of amide protons in the CHARMM force field (HN instead of H) causes g_helix to erroneously fail, as reported on the mailing list.

http://lists.gromacs.org/pipermail/gmx-users/2012-March/069155.html

Mark's fix for #788 works fine for g_hbond, but wouldn't it make sense to standardize nomenclature of these atoms at the .rtp level, as well?

Associated revisions
Revision b76d7b90 - 04/10/2012 03:37 AM - Mark Abraham
Made g_helix sensitive to CHARMM atom naming
Peptide N-H atoms named HN in CHARMM were not recognized as backbone atoms.
Fixes #896
Change-Id: I205b8dc5c895f20e6cde61ee2a1640fc6414b030

Revision b76d7b90 - 04/10/2012 03:37 AM - Mark Abraham
Made g_helix sensitive to CHARMM atom naming
Peptide N-H atoms named HN in CHARMM were not recognized as backbone atoms.
Fixes #896
Change-Id: I205b8dc5c895f20e6cde61ee2a1640fc6414b030

History
#1 - 03/08/2012 11:28 PM - Justin Lemkul
- Assignee deleted (David van der Spoel)

#2 - 03/08/2012 11:28 PM - Justin Lemkul
Standardizing amide H nomenclature within GROMACS would mean coordinate file incompatibility with CHARMM and CHARMM implementations, so generates about as many problems as it might solve. Fix uploaded to gerrit. I don't have a test case - testing would be welcome.

#4 - 04/11/2012 10:55 AM - Rossen Apostolov
I guess we can close this one?

#5 - 04/11/2012 11:43 AM - Mark Abraham
- Status changed from New to Closed