Gromacs - Bug #800

pdb2gmx creates additional incorrect cmap entries

09/01/2011 08:42 AM - Roland Schulz

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: preprocessing (pdb2gmx,grompp)
Target version: 4.5.6

Description
If some non amino acid residue(s) follow(s) the last amino acid, an additional cmap entry is generated. It is centered on the last amino acid and connects to the first N in the non-amino acid residue. The additional residues have to be bonded to the protein (like glycosylation) and thus be in the same segment for the error to occur.

The logic which creates the cmap entries (gen_cmap in pdb2top.c) should either take into account the termini detection (it works correctly in this case) or check that the previous or next residue participating in the cmap entry are protein residues (using residuetypes.dat). Not sure what is the best strategy.

Related issues:
Related to Gromacs - Bug #886: pdb2gmx -cmap needs some mention in manual sec... Closed 02/21/2012

Associated revisions
Revision 4e4d743f - 02/23/2012 02:56 AM - Mark Abraham
Fix pdb2gmx -cmap in corner cases

CMAP torsions are only generated when the atoms are from the same chain (pdb2gmx -merge allows multiple chains to be present in the moleculetype), and their residues are in residuetypes.dat as "Protein".

Fixes #800, #885
Change-Id: Idc4f9a867beedc0be6a4c153606c0731eec86f5f

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I don't have a test case, but I believe [https://gerrit.gromacs.org/#/c/506/] fixes this.

- Status changed from New to Closed

- Category set to preprocessing (pdb2gmx,grompp)
  - Assignee changed from Pär Bjelkmar to Mark Abraham