GROMACS - Bug #2120

gmx do_dssp scount.xvg labels a probability as percent when it is not

02/09/2017 08:48 PM - Chris Neale

Status: Closed
Priority: Low
Assignee: Mark Abraham
Category: analysis tools
Target version: 2016.3
Affected version - extra info:
Affected version: 5.1.2

Description
The -sc scount.xvg output from gmx do_dssp in gmx version 5.1.2 has a final line listing

# SS % ... 

when in fact the numbers sum to 1 and not 100. Since this has existed for a long time (see for example the pasted text from scount.xvg in https://redmine.gromacs.org/issues/683) it probably makes sense to stick with the probabilities byt change the comment from "# SS %" to "# SS prob."

Associated revisions
Revision 12e29c82 - 02/10/2017 02:21 PM - Mark Abraham
Corrected output of gmx do_dssp -sc
This code has always written a probability, and not a percentage, so fixed the label. It still fits within the expected 8-character field.
Fixes #2120
Change-Id: lc3256a3942b2f2375e9f4c0771bbe3afe682acf4

History
#1 - 02/10/2017 02:22 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2120.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~Ic3256a3942b2f2375e9f4c0771bbe3afe682acf4
Gerrit URL: https://gerrit.gromacs.org/6469

#2 - 02/10/2017 02:23 PM - Mark Abraham
- Category set to analysis tools
- Status changed from New to Fix uploaded
- Assignee set to Mark Abraham
- Target version set to 2016.3

Thanks for the report. I did something similar that honours the way things seem to be laid out to fit in 8-character width, so "pr." rather than "prob."

#3 - 02/14/2017 08:17 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 12e29c829e96353092es7bdb37fa7f122f4e19a.

#4 - 03/09/2017 03:47 PM - Mark Abraham
- Status changed from Resolved to Closed