

## GROMACS - Bug #2120

### gmx do\_dssp scout.xvg labels a probability as percent when it is not

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

<b>Status:</b> Closed	
<b>Priority:</b> Low	
<b>Assignee:</b> Mark Abraham	
<b>Category:</b> analysis tools	
<b>Target version:</b> 2016.3	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 5.1.2	

#### Description

The -sc scout.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 scout.xvg in <https://redmine.gromacs.org/issues/683> ) it probably makes sense to stick with the probabilities by 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](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~release-2016~lc3256a3942b2f2375e9f4c0771bbe3afe682acf4

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 [12e29c829e96353092ea7bdb37faf7122f4e19a](#).

##### #4 - 03/09/2017 03:47 PM - Mark Abraham

- Status changed from Resolved to Closed