

## GROMACS - Bug #2544

### gmx rmsf does not fix periodicity in reference structure

06/05/2018 01:56 PM - David van der Spoel

|   |                           |
|---|---------------------------|
| <b>Status:</b> New  |                           |
| <b>Priority:</b> Normal   |                           |
| <b>Assignee:</b> David van der Spoel  |                           |
| <b>Category:</b> analysis tools   |                           |
| <b>Target version:</b> future   |                           |
| <b>Affected version - extra info:</b>   | <b>Difficulty:</b> simple |
| <b>Affected version:</b> 4.0  |                           |
| <b>Description</b>  |                           |
| If the periodicity in the input molecule that is use for fitting is not correct, the fit will be done on a broken molecule leading to incorrect fluctuations. This likely is a left-over from the time when GROMACS did not write broken molecules. |                           |
| <b>Related issues:</b>  |                           |
| Related to GROMACS - Feature #2545: Should grompp fix periodicity of input fi... <b>New</b>   |                           |

### History

#### #1 - 06/05/2018 02:11 PM - David van der Spoel

- File *broken.tpr* added
- File *whole.tpr* added
- File *ub\_traj.pdb* added

To reproduce:

```
gmx rmsf -f ub_traj.pdb -s broken.tpr -res -o rmsf_broken
```

```
gmx rmsf -f ub_traj.pdb -s whole.tpr -res -o rmsf_whole
```

#### #2 - 06/05/2018 02:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2544](#).  
Uploader: David van der Spoel ([spoel@xray.bmc.uu.se](mailto:spoel@xray.bmc.uu.se))  
Change-Id: gromacs~release-2018~lc2b70b3ffc4aa87d1f99b97bc323bcf3d59420ab  
Gerrit URL: <https://gerrit.gromacs.org/7977>

#### #3 - 06/13/2018 12:32 PM - Mark Abraham

- Related to Feature #2545: Should grompp fix periodicity of input files? added

#### #4 - 08/21/2018 10:36 AM - Paul Bauer

- Target version changed from 2018.3 to future

I changed the target version for this, as this involves more general changed to the way the analysis tools work in the end.

### Files

|             |        |            |                     |
|-------------|--------|------------|---------------------|
| broken.tpr  | 592 KB | 06/05/2018 | David van der Spoel |
| whole.tpr   | 592 KB | 06/05/2018 | David van der Spoel |
| ub_traj.pdb | 190 KB | 06/05/2018 | David van der Spoel |