

GROMACS - Task #2889

update grompp warnings for brevity, usefulness and actionability

03/11/2019 02:15 PM - Mark Abraham

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| Status: | New | |
| Priority: | Normal | |
| Assignee: | Mark Abraham | |
| Category: | preprocessing (pdb2gmx,grompp) | |
| Target version: | 2020 | |
| Difficulty: | simple | |
| Description | | |
| <p>We intend grompp to issue warnings when the user is doing something that is likely to be inconsistent with modelling physics. We have feedback (often vague) that things are hard to use.</p> <p>Naturally users report "grompp was hard to use" when the actual issue is any of</p> <ul style="list-style-type: none">• I didn't know what this warning meant,• I mis-edited the .top file,• I didn't know where to find the docs,• I misunderstood the docs,• grompp warned about something that is fine in my sub-case,• grompp also told me about things I don't understand,• grompp also told me about things I understand but would never act upon, and doubtless many others. <p>We should go through our warning messages and improve (or eliminate) them. One suggestion is that they should be at most two lines, but provide enough clue why the warning is (or is not) something worth heeding, and perhaps where to go for more information to make a decision.</p> | | |