

GROMACS - Feature #2036

gmx solvate should work with molecules

08/19/2016 03:02 PM - David van der Spoel

Status:	Closed
Priority:	Normal
Assignee:	
Category:	preprocessing (pdb2gmx,grompp)
Target version:	2018
Difficulty:	simple
Description	
<p>gmx solvate can not handle molecules as solvent. According to the documentation it uses the residue number in the input file, ("In practice this means that two subsequent solvent molecules in the solvent coordinate file should have different residue number.") but this is not entirely correct since the residue names are interpreted as well. As a result a molecule containing more than one residue with different names (even if they have the same residue number) is torn apart by gmx solvate.</p> <p>The obvious solution would be to use real the molecule information in a tpr file.</p>	

History

#1 - 08/19/2016 06:53 PM - Teemu Murtola

It interprets residues exactly like every other Gromacs program, but the help text hasn't been updated to match the new implementation that also considers residue names.

A workflow that would require a tpr file as solvent would not be particularly practical, either.

#2 - 08/19/2016 06:57 PM - David van der Spoel

I agree a tpr file is a hassle, however now it is impossible to dissolve a protein into a solution containing other molecules. In fact the code already reads tpr files and extracts topologies, so it will not be too hard to fix.

#3 - 08/19/2016 07:24 PM - Teemu Murtola

Note that if we want to really use gmx_mtop_t everywhere, the whole tool and the helpers it uses needs to be rewritten to not use t_atoms, and that will also probably solve this. Doing something else is likely to waste significant effort (since you would need to make the helpers aware of molecules, in a way that is not compatible with gmx_mtop_t).

#4 - 08/19/2016 07:44 PM - Teemu Murtola

I would also argue that the behavior that would fit into a typical workflow would be that the tool would read the molecule types from the .top file given as input (if present) and recognize those from the structure file.

#5 - 08/23/2016 03:25 PM - David van der Spoel

In fact gmx insert-molecules can work as stand-in for the desired functionality, it can even insert whole proteins. So no need for this feature.

#6 - 08/23/2016 03:25 PM - David van der Spoel

- Status changed from New to Closed