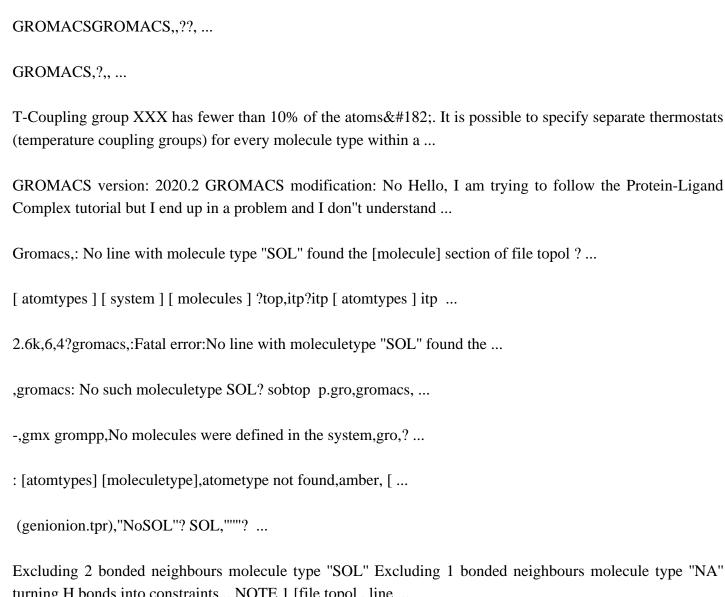
## **SOLAR** Pro.

## Fatal error molecule type sol contains no atoms gromacs



turning H bonds into constraints... NOTE 1 [file topol , line ...

Fatal error: No such moleculetype XXX¶ Each type of molecule in your [molecules] section of your top file must have a corresponding [moleculetype] section defined previously, ...

Fatal error: There were 4 missing atoms in molecule Protein\_chain\_A, if you want to use this incomplete topology anyhow, use the option -missing \*.pdb\*.rtp ...

I ran gromacs with command: grompp -f ions.mdp -c protein a\_solv.gro -p topol -o ions.tpr. and yielded a Fatal error: Correct the number of coordinates in coordinate file (protein a.gro, 36891 ...

## **SOLAR** Pro.

## Fatal error molecule type sol contains no atoms gromacs

No default Proper Dih. types. ERROR 2 [file sin p, line 344]: No default Proper Dih. types. Excluding 3 bonded neighbours molecule type "Protein\_chain\_A" Excluding 3 ...

Fatal error: No such moleculetype XXX# Each type of molecule in your [molecules] section of your top file must have a corresponding [moleculetype] section defined previously, ...

Solvent box contains 99373 atoms in 28208 residues Removed 12253 solvent atoms due to solvent-solvent overlap Removed 5122 solvent atoms due to solute-solvent ...

However, after the solvation stage, I keep encountering this error when I try to run the command: "gmx grompp -f ions.mdp -c solvated.gro -p topol -o ions.tpr" The error: ...

I am facing a problem between different versions of gromacs for gmx pdb2gmx. I have a protein-ligand system, I did all the necessary steps mentioned in gromacs manual for ...

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