GROMACS - Bug #2580

sc-coul option yields different free energy estimate on a ligand with zero partial charge

07/19/2018 06:49 PM - zhiyi wu

Status:	Feedback wanted		
Priority:	High		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018.3		

Description

I'm trying to calculate the free energy difference of decoupling the vdw interactions of ligand from the water. For simplicity, the ligand bears no partial charge.
Since the ligand has no partial charge, turning on the softcore Columbic interaction shouldn't have any effect on the free energy of decoupling the vdw part of the ligand.
However, the free energy difference calculated on the same trajectory yields 1.216kcal/mol when sc-coul=yes and -0.428 kcal/mol when sc-coul=no.

The traj folder contains all the trajectory, while sc_coul_on and sc_coul_off contains the mdp file, tpr file and dhdl file in both sc-coul=yes and sc-coul=no. The dhdl file can be reproduced from the trajectory by running run.sh.
Since the trajtory is very large, the file is shared by google drive.

https://drive.google.com/file/d/18ELypM_TaINYJzx0kwWizfliSAxfxR7F/view?usp=sharing

History

#1 - 09/11/2018 08:10 AM - Berk Hess

- Status changed from New to Feedback wanted

Does the fix for #2640 also fix this issue as well as #2573 ?