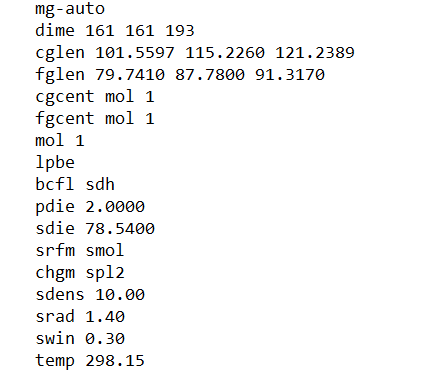
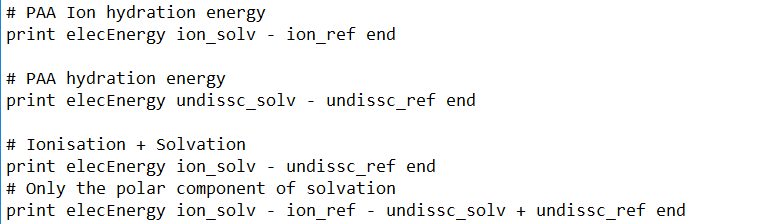
Results of PAA simulations

# August 7th

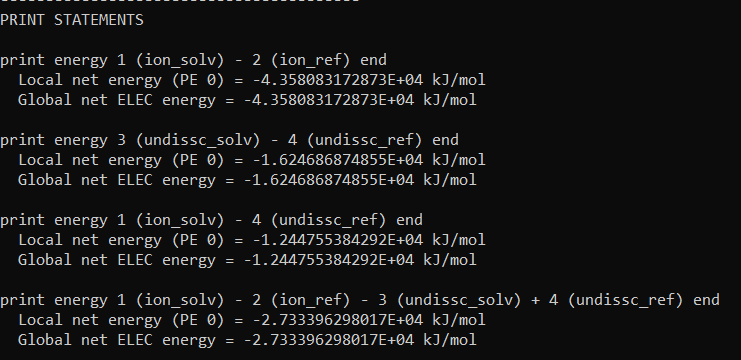
## Multigrid method

### Method:





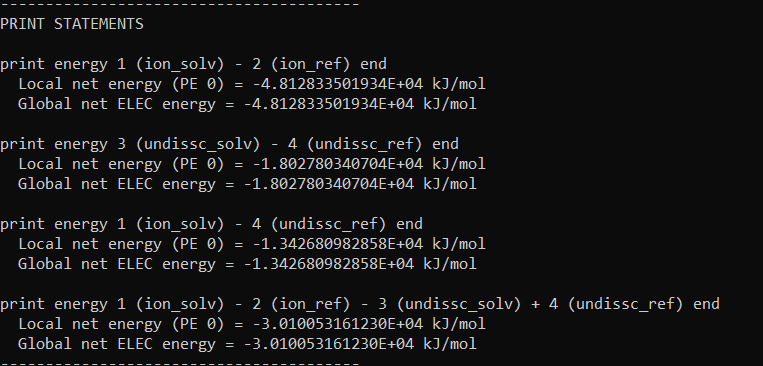
### Calculations:

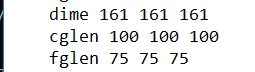


Polar Solvation energy = -2.733\*104 kJ/mol

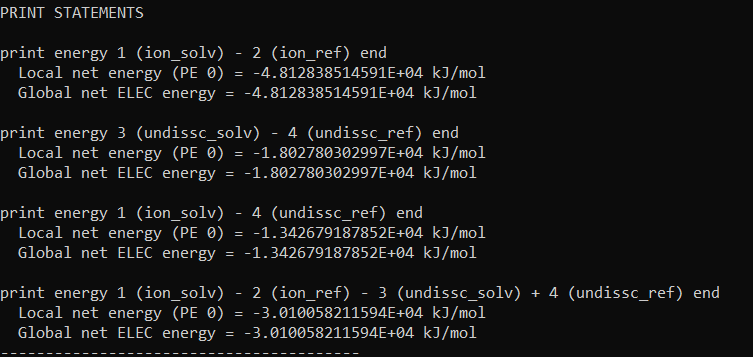
Total solvation free energy = -1.244755\*104 kJ/mol

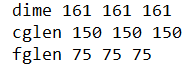
## Multigrid 2





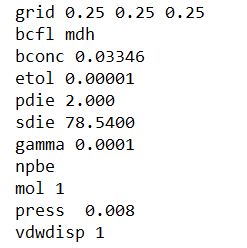
## Multigrid 3



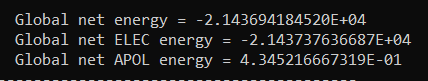


## Geometric Flow Solvation

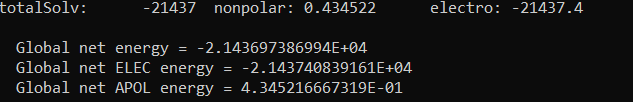
### Method: molecule chosen: pdb with ions



### Results:

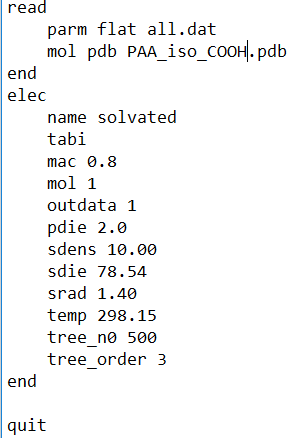


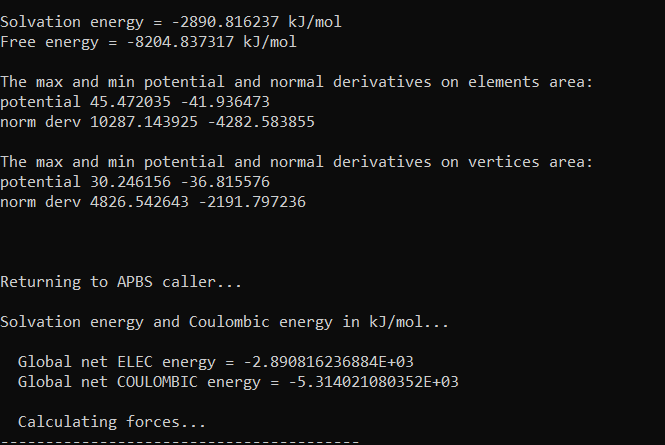
**After decreasing etol to 0.000001**



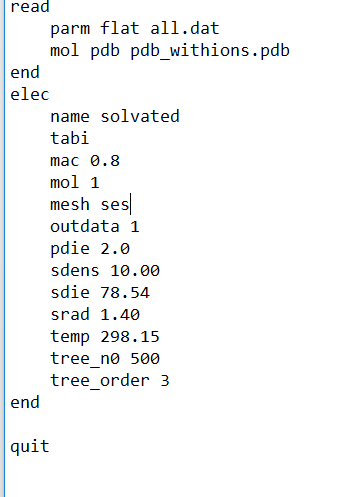
## TABI

**Solvation energy and free energy of undissociated PAA**

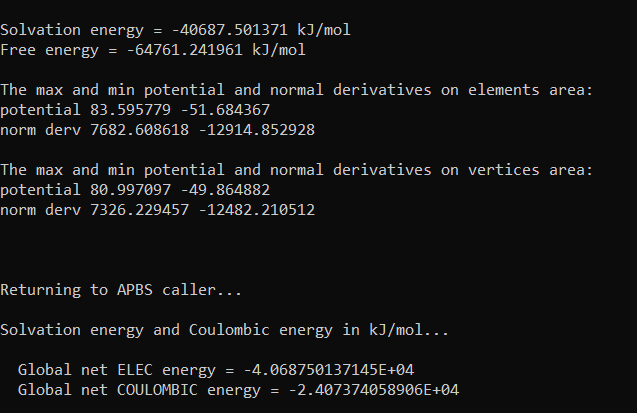




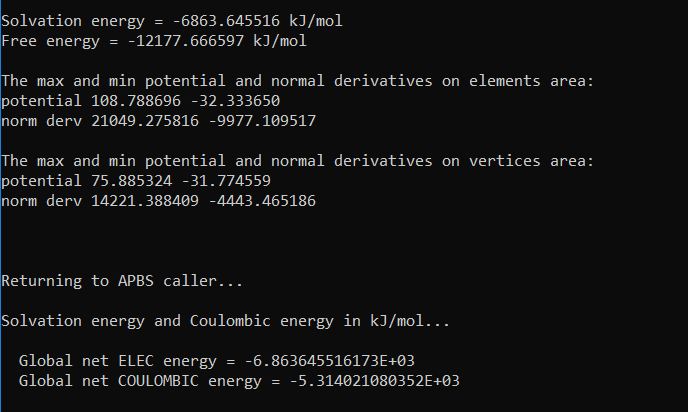
**Solvation and free energy of dissociated PAA**



**Used SES Nanoshaper**



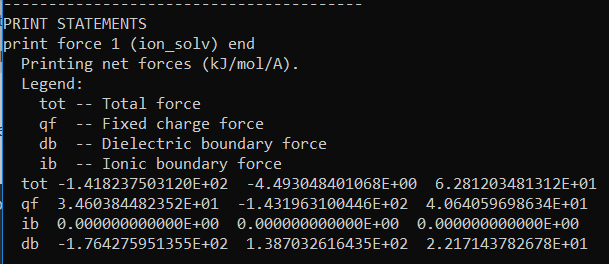
**Solvation energy and free energy of undissociated PAA using SES Nanoshaper**

****

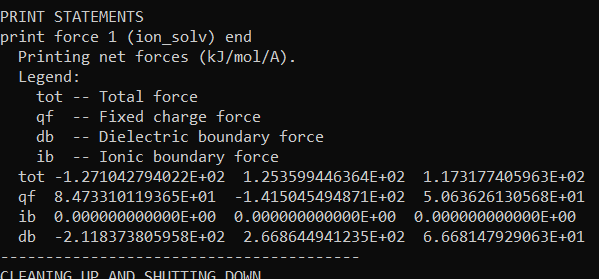
**Therefore, Polar solvation energy = -4\*10^4+6.86\*10^3 = -3.382\*10^4**

# August 10th

## Force calculations using spl2 srfm, npbe, multigrid for ion with Na+

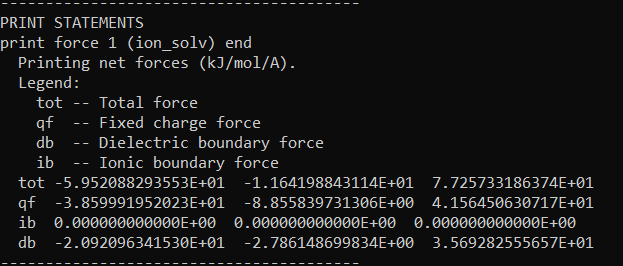


**Srfm spl4 calculation**

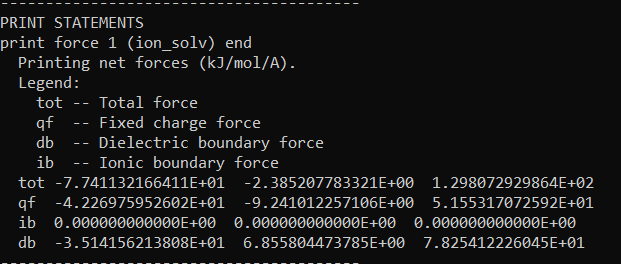


## Similar force calc for undiss PAA

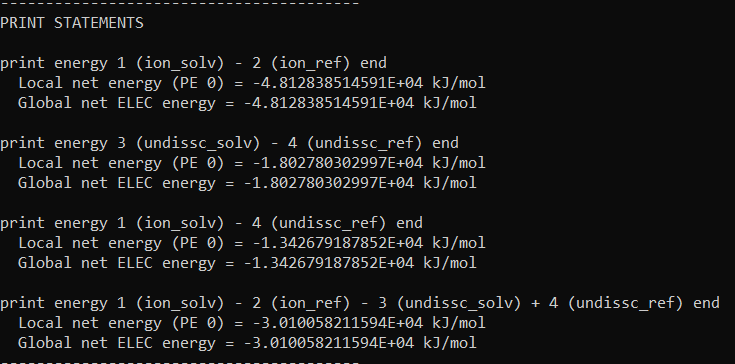
**Srfm spl2**



**Srfm spl4**

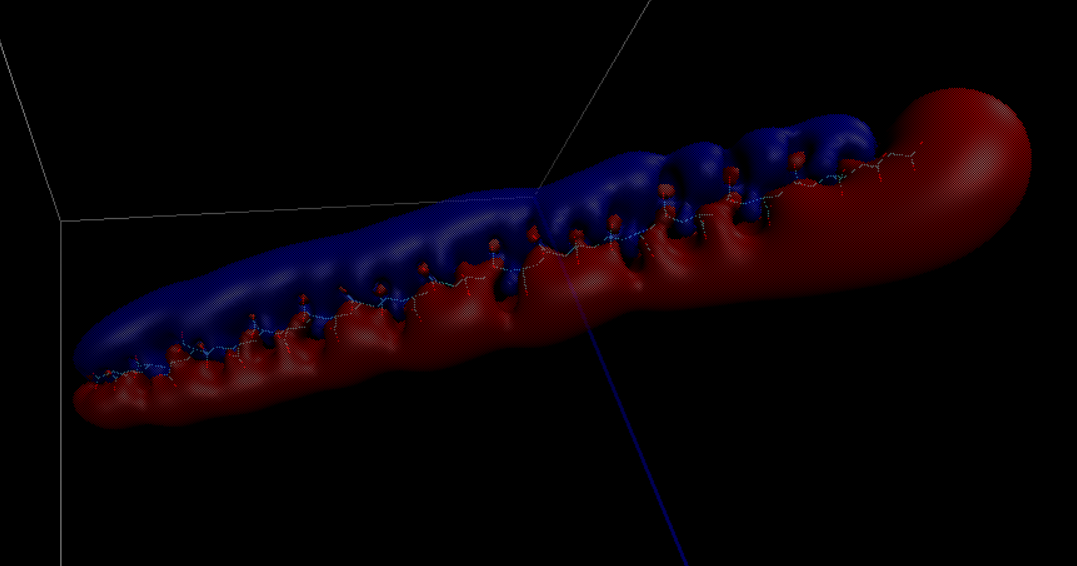


## Solvation with npbe

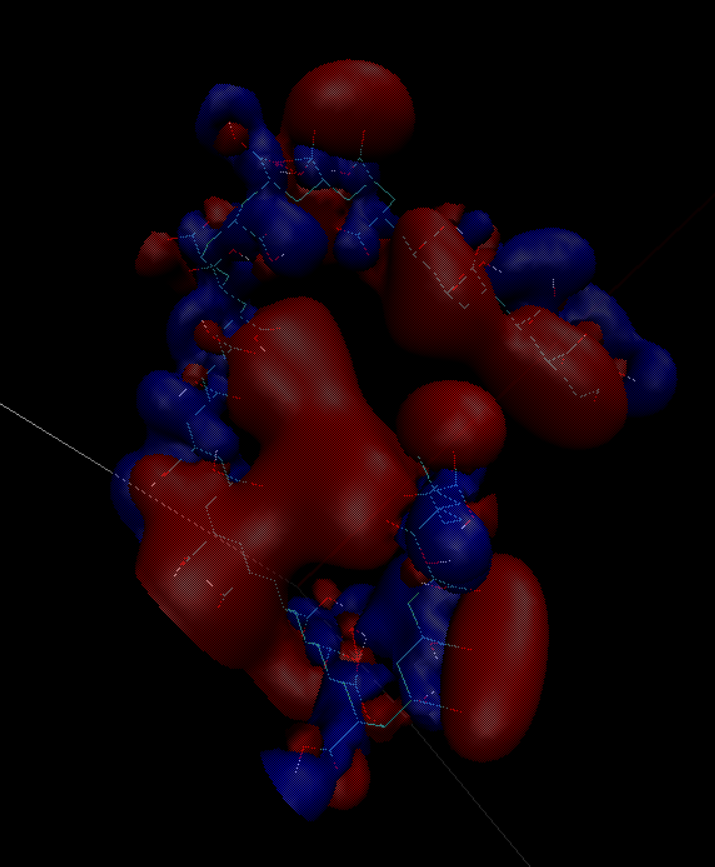


## Surface potentials

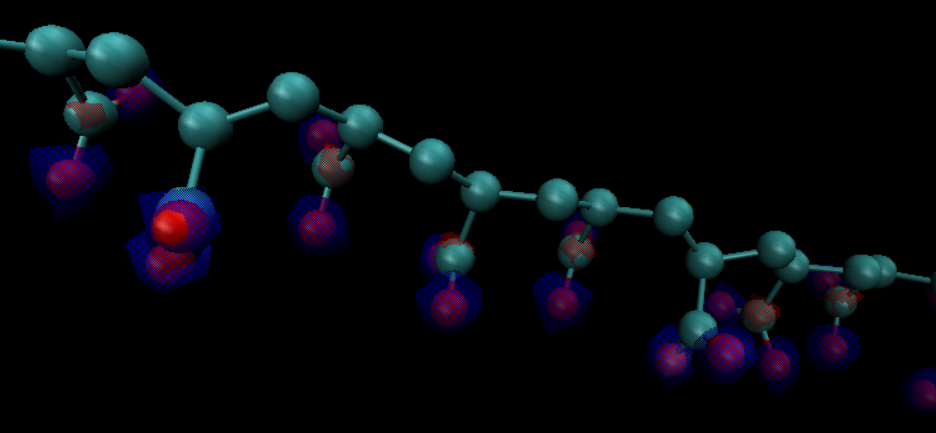
### Charged PAA with ions



### Uncharged PAA



### Charged PAA without ions



# Update 11/06/2021

Noticed that C1-C3 interchanged in pdb/dat file. So swapped their values in dat file. New simulation for hydration energy gives similar results.

