GROMACS - Feature #2956

SAXS resolution

05/17/2019 09:58 AM - Vitaly Kocherbitov

Status:	New	
Priority:	Normal	
Assignee:		
Category:		
Target version:		
Difficulty:	simple	

Description

Hi!
I tried to calculate SAXS scattering corves using gmx saxs. It works but it is impossible to change resolution. The output (q values in nm-1) has a resolution of 1 point per 1 nm-1, which is very poor. I tried to limit the output range by using the -startq and -endq options hoping to get better resolution in a narrow range, but it still gives the same poor resolution and only cuts the the length of output data. Would it be possible to introduce an option for changing the q resolution?
Thank you!