

TNG trajectory library - Feature #1229

Selection groups

04/24/2013 09:30 AM - Magnus Lundborg

Status:	Resolved	
Priority:	Normal	
Assignee:	Magnus Lundborg	
Category:		
Target version:	version 1	
Description		
Add support for commonly used selection groups (protein, water, ions, etc.).		

History

#1 - 10/25/2013 09:21 AM - Magnus Lundborg

The actual groups can either be written as separate molecules, which is not elegant, or perhaps just by using particle mapping blocks to map the relevant particles so that they can be written in sequence.

Later on it would be good to have a selections block after the molecules block.

#2 - 10/25/2013 09:22 AM - Magnus Lundborg

- Target version changed from version 2 to version 1

#3 - 11/29/2013 04:38 PM - Magnus Lundborg

- Status changed from New to Resolved

Now it's written as separate molecules. It works, but can be improved later on.