GROMACS - Bug #2848

gmx make_ndx ignores last residue in case only CA's are present in GRO file

01/30/2019 06:16 AM - Floris van Eerden

Status:	New		
Priority:	Normal		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018		

Description

When I want to generate an index file of a gro file that only contains the CA atoms of a protein, gmx make_ndx does not list the last residue when using the 'l' command. It does however write the residue out, if you select its residue index number (ri option)
I noticed that gmx make_ndx does recognize the last residue in case I leave the amino acid N in the file.

To summarize:
gmx make_ndx does not list last residue in a CA only file.

Files

withN.gro	8.4 KB	01/30/2019	Floris van Eerden
NO_N.gro	8.36 KB	01/30/2019	Floris van Eerden