Core dump with gmx rdf with some selections

Description
When running some selections with gmx rdf 2019.2 get:
'Segmentation fault (core dumped)'

Exact same files and command, but using 2016.3 the program executes fine.

```
gmx rdf -f md_001_short.xtc -s md_001.tpr -bin 0.01 -n index.ndx -seltype part_res_com -selrpos part_res_com -o ' Select 11 and 11

'gmx rdf -f md_001_short.xtc -s md_001.tpr -bin 0.01 -n index.ndx -seltype dyn_res_com -selrpos dyn_res_com -o ' Select 11 and 11

This one works fine with 2019.2:
'gmx rdf -f md_001_short.xtc -s md_001.tpr -bin 0.01 -n index.ndx -seltype whole_res_com -selrpos whole_res_com -o'
```

Associated revisions
Revision a822b10a - 06/11/2019 02:55 PM - Paul Bauer
Fix residue and molecule indexing in selections

The residue and molecule indexing did not account for the global indices when building blocks from selections.

Also fixed a docs formatting issue noticed while working on the fix.

Fixes #2951
Change-Id: Ifa16f032822f5d96b6ff747333a7aed60b9a414d

Revision 6d0ed8b7 - 07/05/2019 10:09 AM - Mark Abraham
Improve tests of index block construction

Only trivial topologies were tested, and bugs have been identified. Some test code is commented out until the fix lands.

Added missing Doxygen

Improved some assertions hit while investigating the issue.

Refs #2951
Change-Id: Ia03e38aca42be43efa1fd548c32e522d97e13e94

History
#1 - 05/14/2019 12:04 PM - Paul Bauer
- Status changed from New to Accepted

I reproduced this.
The bug got introduced in b2b1088c3726cea7a5e696e11c81dfab8f82fe8d
#2 - 05/14/2019 02:55 PM - Paul Bauer
- Status changed from Accepted to Fix uploaded

#3 - 05/14/2019 02:55 PM - Paul Bauer
- Target version set to 2019.3

#4 - 06/11/2019 02:57 PM - Mark Abraham
- Status changed from Fix uploaded to Closed

Files

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