

**S1Table.** The details of performed MD simulations

|                       |                                 |   |
|-----------------------|---------------------------------|---|
| Set No.               | 1                               | 2   |
| Protein variants      | WT and 3GLU                     | WT, 2GLU and 3GLU   |
| Goal                  | Investigation of ion entry path | Determination of the ability of the protein to hold the ion in a predetermined position |
| Time [ns]             | 150                             | 100   |
| C <sub>NaCl</sub> [M] | 2                               | 0.15  |