|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Force Field#** | **Gate** | **Cβ-Cβ distance (Å)** | **Pore radius (Å)** | **Water density (Å-1)** |
| AMBER | I398 | 12.76 ± 2.97 | 0.95 ± 0.20 | 7.03 x 10-3 |
| I398N | 10.70 ± 1.00 | 2.13 ± 0.47 | 1.33 x 10-2 |
| CHARMM36m | I398 | 15.21 ± 1.35 | 3.10 ± 0.33 | 1.20 x 10-2 |
| I398N | 12.04 ± 1.10 | 2.98 ± 0.57 | 1.95 x 10-2 |

#Average properties were determined over 10μs of simulation.