**Table S1**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **#** | **[protein] (mM)** | **N peptides** | **[salt] (M)** | **force field** | **electrostatics** | **t (ns)** | **# atoms** | **N simulations** | **RMSD (Å)** | **# alpha** | **dPHE (Å)** |
|  |  |  |  |  |  |  |  |  | (wt. | car.) | (wt. | car.) | (wt. | car.) |
| **1** | 9.2 | 8 | 0 | GROMOS45a3 | RF | 50 | ∼140,000 | 3 | 2.7 ± 1.1 | 8.2 ± 0.8 | 22.6 ± 1.9 | 6.3 ± 3.8 | 19.9 ± 1.7 | 34.9 ± 2.3 |
| **2** | 6 | 4 | 0.05 | GROMOS45a3 | RF | 50 | ∼110,000 | 3 | 2.4 ± 0.8 | 8.5 ± 0.7 | 22.9 ± 1.5 | 5.3 ± 2.0 | 20.3 ± 1.7 | 38.2 ± 3.4 |
| **3** | 6 | 4 | 0.1 | GROMOS45a3 | RF | 50 | ∼110,000 | 3 | 2.8 ± 1.8 | 8.4 ± 0.6 | 22.6 ± 1.9 | 6.2 ± 3.2 | 19.5 ± 1.0 | 37.5 ± 3.6 |
| **4** | 6 | 4 | 0.2 | GROMOS45a3 | RF | 50 | ∼110,000 | 3 | 2.2 ± 0.5 | 8.1 ± 0.6 | 23.0 ± 1.4 | 6.6 ± 3.0 | 20.7 ± 1.6 | 33.5 ± 6.0 |
| **5** | 6 | 4 | 0.4 | GROMOS45a3 | RF | 100 | ∼110,000 | 3 | 2.5 ± 0.8 | 8.3 ± 0.6 | 22.7 ± 1.8 | 6.7 ± 2.7 | 19.5 ± 1.9 | 38.1 ± 6.0 |
| **6** | 6 | 4 | 0.8 | GROMOS45a3 | RF | 100 | ∼110,000 | 3 | 2.7 ± 1.3 | 8.1 ± 0.6 | 22.4 ± 2.0 | 6.1 ± 3.0 | 19.5 ± 1.3 | 32.5 ± 4.5 |
| **7** | 6 | 4 | 0 | GROMOS54a7 | RF | 100 | ∼110,000 | 1 | 3.8 ± 3.0 | 8.6 ± 1.0 | 22.6 ± 2.1 | 7.7 ± 2.3 | 19.9 ± 1.2 | 41.8 ± 10.2 |
| **8** | 6 | 4 | 0.05 | GROMOS54a7 | RF | 100 | ∼110,000 | 1 | 4.3 ± 2.5 | 8.0 ± 0.6 | 22.4 ± 2.4 | 6.6 ± 4.6 | 19.0 ± 1.0 | 34.3 ± 3.4 |
| **9** | 6 | 4 | 0.05 | GROMOS45a3 | PME | 200 | ∼110,000 | 3 | 2.8 ± 0.8 | 7.9 ± 0.8 | 20.7 ± 3.2 | 6.4 ± 3.7 | 20.9 ± 3.2 | 29.0 ± 3.7 |
| **10** | 6 | 4 | 0.05 | GROMOS54a7 | PME | 200 | ∼110,000 | 3 | 2.4 ± 0.5 | 7.8 ± 0.9 | 23.1 ± 1.5 | 9.1 ± 5.0 | 21.2 ± 2.9 | 30.7 ± 4.0 |
| **11** | 6 | 4 | 0.05 | AMBER99SB -ILDN | PME | 200 | ∼110,000 | 3 | 2.2 ± 0.4 | NA | 21.4 ± 2.0 | NA | 18.6 ± 0.8 | NA |
| **12** | 6 | 4 | 0.05 | CHARMM22-CMAP | PME | 200 | ∼110,000 | 3 | 2.4 ± 0.5 | NA | 23.1 ± 1.3 | NA | 18.6 ± 0.6 | NA |
| **aggregate average (GROMOS force fields only)** | | | | | | | | | 2.7 ± 1.2 | 8.1 ± 0.8 | 22.3 ± 2.3 | 7.0 ± 3.9 | 20.3 ± 2.4 | 33.3 ± 5.8 |
| **Ref [31]** | ∞-1 | 1 | 0 | GROMOS45a3 | RF | 110 | ∼14,000 | 5 | 3.1 ± 1.4 | 7.3 ± 0.9 | 21.8 ± 3.2 | 12.1 ± 5.1 | 19.3 ± 1.4 | 29.3 ± 5.3 |