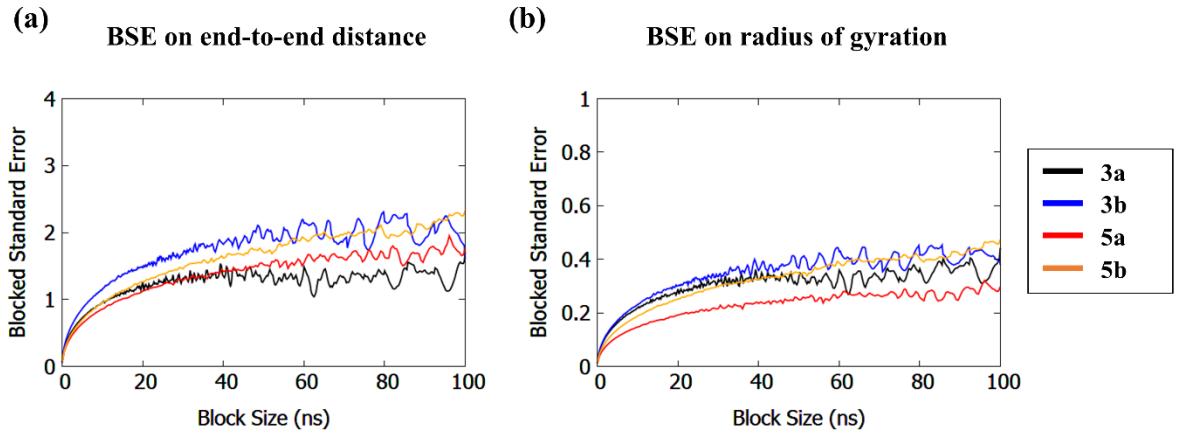
## Simulation Convergence




*Supplementary Figure S1: Block averaging analysis for the (a) end to end distance,* r*, and (b) radius of gyration for 6 RUs of the serogroup 3 and 5 O-Ags. The plot of blocked standard error (BSE) versus block size reaches a plateau for all the O-Ags of serogroup 3 and 5, indicating convergence in each simulation.*

| | 1A_2B | 1A_1D | 2A_1D | 2A_1F | 3A_1F | 1B_2C | 1B_3C | 1C_3D | 2C_5B | 1D_1F |
|---|---|---|---|---|---|---|---|---|---|---|
| Average distance[a] | 2.3 ± 0.2 | 3.9 ± 0.3 | 2.3 ± 0.2 | 2.3 ± 0.3 | 2.7 ± 0.3 | 3.7 ± 0.6 | 2.3 ± 0.2 | 2.2 ± 0.2 | 2.7 ± 0.4 | 2.8 ± 0.5 |
| $r^6$ average MD[a] | 2.3 ± 0.2 | 3.8 ± 0.6 | 2.2 ± 0.2 | 2.3 ± 0.2 | 2.6 ± 0.3 | 3.3 ± 0.8 | 2.2 ± 0.2 | 2.2 ± 0.1 | 2.5 ± 0.3 | 2.6 ± 0.4 |
| Theillet NMR[b] | 2.2 ± 0.1 | 3.7 ± 0.4 | 2.3 ± 0.1 | 2.3 ± 0.1 | 2.4 ± 0.2 | 3.3 ± 0.4 | 2.2 ± 0.1 | 2.3 ± 0.1 | 2.7 ± 0.3 | 2.6 ± 0.2 |
| Theillet MD[b] | 2.3 | 3.5 | 2.4 | 2.3 | 2.4 | 3.3 | 2.2 | 2.3 | 2.7 | 2.6 |

*Supplementary Table S1: Comparison between MD simulation and experimental data of distances between hydrogen atom pairs (columns) are in good agreement for serotype 3a. (a) The mean distance and corresponding $r^6$ average from our 1.2 µs production runs, excluding 200 ns for equilibration. (b) Experimental NMR distances from NOE build-up curves (estimated 10% error) of the native O-Ag and distances calculated by full ensemble relaxation analysis of 60 ns MD simulations of a 3RU serotype 3a O-Ag (Theillet et. al., 2010).*

| | 1A_1B | 1A_2B | 1A_4B | 1A_1D | 1A_2D | 2A_1B | 2A_1D | 2A_2D | 2A_5D | 2A_1G | 4A_1D | 5A_1B | 5A_2B | 1B_2C | 1B_3C | 1B_4C | 2B_4C | 2B_1G | 3B_1G | 3B_5G |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Average distance[a] | 3.6 ± 0.6 | 2.3 ± 0.2 | 4.2 ± 0.4 | 3.6 ± 0.7 | 4.4 ± 0.3 | 5.0 ± 0.2 | 2.4 ± 0.2 | 4.3 ± 0.2 | 4.0 ± 0.4 | 4.5 ± 0.8 | 4.2 ± 0.4 | 2.6 ± 0.4 | 3.7 ± 0.5 | 4.0 ± 0.4 | 2.3 ± 0.2 | 3.9 ± 0.3 | 4.2 ± 0.3 | 2.4 ± 0.5 | 2.7 ± 0.3 | 3.0 ± 0.6 |
| $r^6$ average[a] | 3.2 ± 0.8 | 2.2 ± 0.2 | 4.0 ± 1.1 | 3.1 ± 0.8 | 4.3 ± 0.4 | 4.9 ± 0.2 | 2.3 ± 0.2 | 4.3 ± 0.8 | 3.9 ± 0.4 | 3.9 ± 1.4 | 4.0 ± 0.8 | 2.4 ± 0.3 | 3.4 ± 0.9 | 3.6 ± 1.5 | 2.3 ± 0.2 | 3.7 ± 1.1 | 4.1 ± 0.4 | 2.3 ± 0.2 | 2.6 ± 0.4 | 2.7 ± 0.4 |
| ROE[b] | 3.1 ± 0.3 | 2.1 ± 0.2 | 4.7 ± 0.5 | | 4.5 ± 0.4 | | 2.0 ± 0.2 | 4.5 ± 0.4 | 4.1 ± 0.4 | 4.1 ± 0.4 | 4.2 ± 0.4 | 2.4 ± 0.2 | 4.6 ± 0.5 | 3.4 ± 0.3 | 2.1 ± 0.2 | 4.3 ± 0.4 | 4.6 ± 0.5 | 2.3 ± 0.2 | 2.5 ± 0.2 | 3.0 ± 0.3 |
| NOE[b] | 3.0 ± 0.3 | 2.1 ± 0.2 | 4.6 ± 0.5 | 3.5 ± 0.3 | | 4.7 ± 0.5 | 2.1 ± 0.2 | 4.5 ± 0.4 | 3.8 ± 0.4 | 4.1 ± 0.4 | 4.3 ± 0.4 | 2.6 ± 0.3 | 4.3 ± 0.4 | 2.9 ± 0.3 | 2.1 ± 0.2 | 4.4 ± 0.4 | 4.8 ± 0.5 | 2.4 ± 0.2 | 2.2 ± 0.2 | |
| Theillet MD[c] | 3.2 | 2.3 | 4.5 | 3.2 | | 4.9 | 2.3 | 4.5 | 4.1 | 4.0 | 4.2 | 2.4 | 3.9 | 3.3 | 2.3 | 4.0 | 4.4 | 2.3 | 2.6 | |

*Supplementary Table S2: Distances of pairs of hydrogen atoms (columns) from MD simulation and experimental data for serotype 5a. (a) The average distance and corresponding $r^6$ average from our 2 µs production runs, excluding 200 ns for equilibration. (b) Experimental NMR distances (estimated 10% error) derived from NOE build-up curves and ROESY off-resonance measurements on the native O-Ag sample with an avDP15 (Clement et. al., 2003). (c) Distances calculated by full ensemble relaxation analysis of 60 ns MD simulations of a 3RU O-Ag (Theillet et. al., 2010).*