Table S1. The C_{α} root mean-square deviation (RMSD) of ligand-free TLR4-MD2 heterodimer, (TLR4-MD2)$_2$ tetramer, lipopolysaccharide (LPS)-bound (TLR4-MD2)$_2$ tetramer, and neoseptin3-bound (TLR4-MD2)$_2$ tetramer complexes are averaged over the last 1.0 μs of each trajectory. Trajectories in each complex are identified with a number from 1 to 4 (#) and their average is denoted by '1-4' as shaded in light grey. The values in parenthesis are standard deviation.

Complex	#	*RMSD*
(TLR4-MD2)	1	**3.82** (0.95)
(TLR4-MD2)	2	**2.81** (0.53)
(TLR4-MD2)	3	**3.40** (0.54)
(TLR4-MD2)	4	**4.05** (0.62)
(TLR4-MD2)	1-4	**3.52** (0.55)
(TLR4-MD2)$_2$	1	**4.33** (0.46)
(TLR4-MD2)$_2$	2	**3.07** (0.32)
(TLR4-MD2)$_2$	3	**4.24** (0.83)
(TLR4-MD2)$_2$	4	**4.10** (0.46)
(TLR4-MD2)$_2$	1-4	**3.93** (0.58)
(TLR4-MD2-LPS)$_2$	1	**2.44** (0.36)
(TLR4-MD2-LPS)$_2$	2	**2.69** (0.38)
(TLR4-MD2-LPS)$_2$	3	**2.68** (0.49)
(TLR4-MD2-LPS)$_2$	4	**2.25** (0.28)
(TLR4-MD2-LPS)$_2$	1-4	**2.51** (0.21)
(TLR4-MD2-neoseptin3)$_2$	1	**2.86** (0.40)
(TLR4-MD2-neoseptin3)$_2$	2	**3.13** (0.28)
(TLR4-MD2-neoseptin3)$_2$	3	**2.87** (0.39)
(TLR4-MD2-neoseptin3)$_2$	4	**2.88** (0.42)
(TLR4-MD2-neoseptin3)$_2$	1-4	**2.93** (0.13)