Martini Force Field Parameters for Glycolipids

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Published in:
Journal of Chemical Theory and Computation

DOI:
10.1021/ct3009655

Publication date:
2013

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Supporting information

Alternative model for MGDG, SQDG and DGDG

In developing glycolipid models we tested many different mapping schemes and bonded parameter sets. Most of these were abandoned at some point for one reason or another, but we kept working on an additional model for MGDG, SQDG, and DGDG. This alternative model is described in detail here. Compared to the model presented in the main manuscript, the alternative model is slightly less accurate in reproducing the properties of the respective glycolipids at the atomistic level, but has the important advantage of running stable with much larger time steps up to 40 fs.

The mapping of the alternative model for MGDG, SQDG, and DGDG is shown in Figure S1. Compared to the standard mapping (Fig. 2A-C), the inclusion of part of the glycerol linkage in the beads of the glycolipid head group is the most noticeable difference. Based on this mapping, bonded parameters were derived by the standard procedure of fitting CG probability distributions of the given parameter onto the probability distribution from the atomistic simulation as explained in the main text. To be able to preserve a time-step of at least 20 fs, the probability distributions for dihedral angles were not considered, i.e. no dihedral angle potential was used. In the later stage of parametrization, the focus shifted to reproducing the area per lipid and membrane thickness obtained for the atomistic systems. This was mainly achieved through changes in bead type and by introducing small bead types, analogous to the procedure described in the main text. The final set of bonded parameters is given in Table S1. A comparison of key angle distributions between the CG model and the reference all-atom model is shown in Fig. S2. Key properties of the alternative model are summarized in Table S2.

Structural conformation of GM1 and DGDG in solution

As mentioned in the main manuscript, simulations of different glycolipid head groups were carried on for their structural characterization in solution. We present here the complementary set of RDFs for the head groups corresponding to GM1 (Figure S3) and DGDG (Figure S4). For a description of the simulation set up, please refer to Methods in the main manuscript.

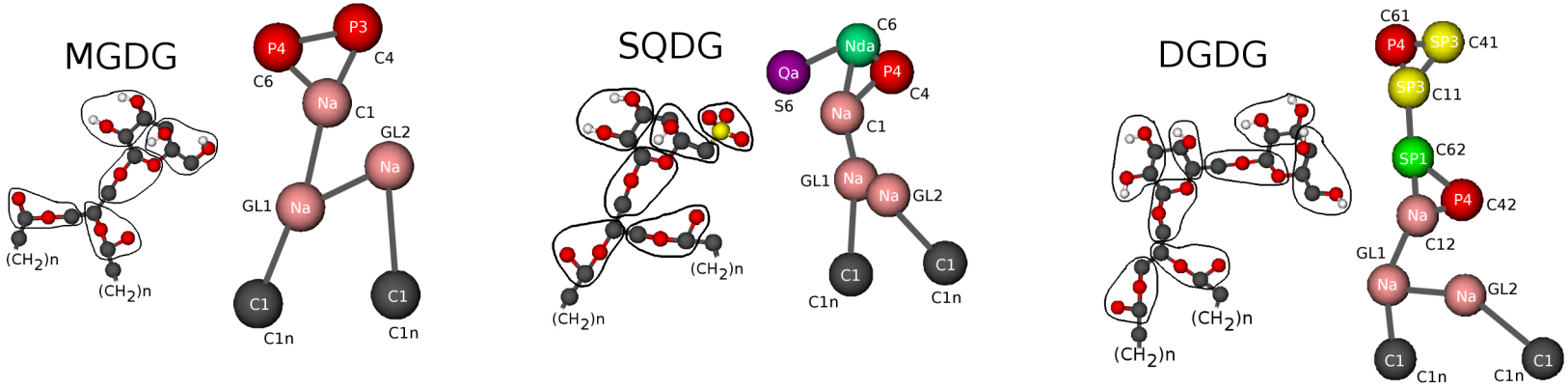

Figure S1. Alternative mapping of the glycolipids MGDG, SQDG, and DGDG. CG bead types and bead labels are indicated. Compare to Figure 2A-C in the main manuscript.

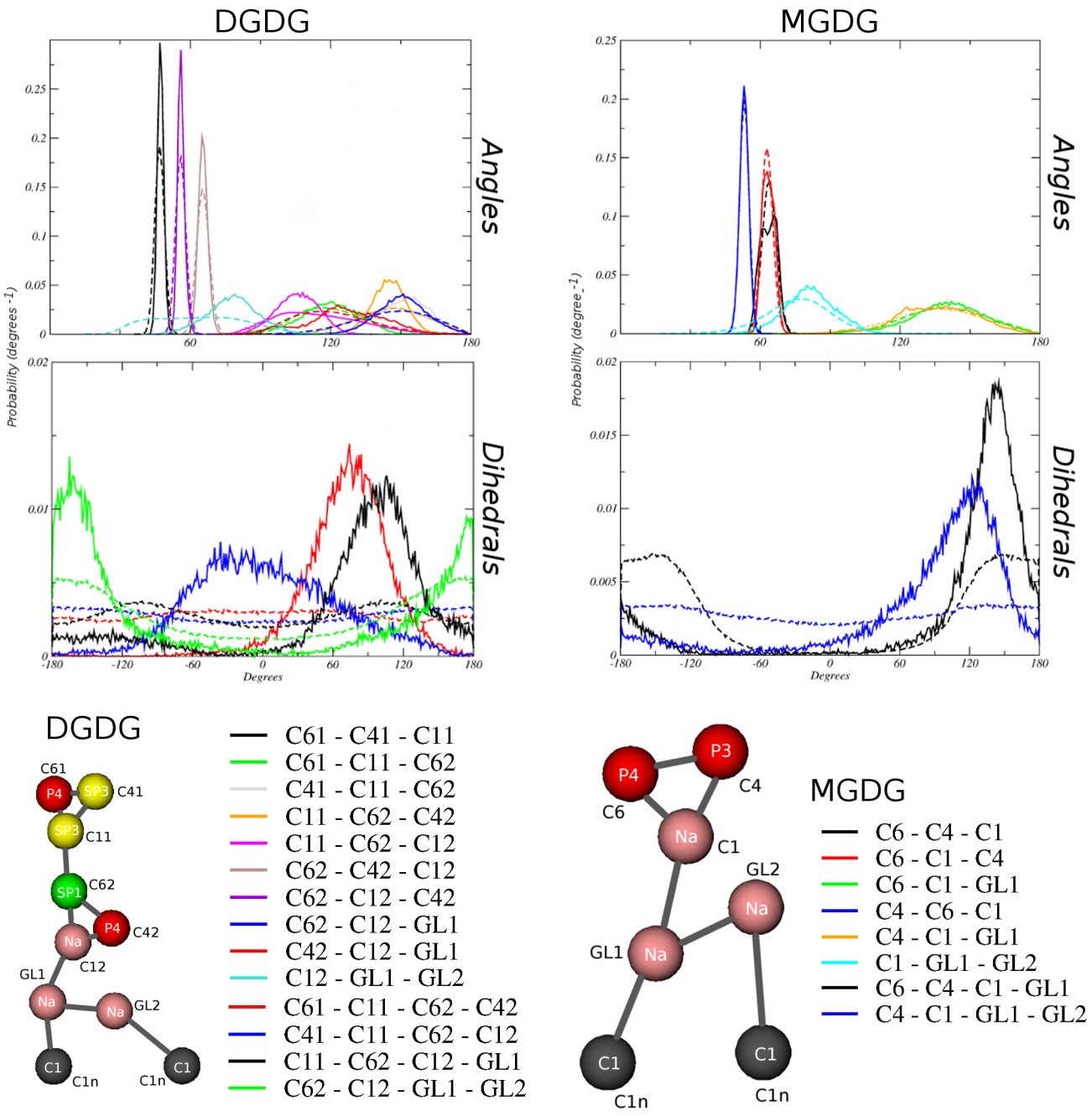

Figure S2. Top: angle and dihedral angle distributions for selected beads in DGDG and MGDG lipid membranes. Solid lines are used for distributions obtained from reference all-atom simulations, dotted beads are obtained with the CG model. Bottom: color coding of the respective angle and dihedrals for which the distributions are shown. Note: dihedral angle potentials were not explicitly added in this model.

Glycolipid	Bonds	R_{bond}	K_{bond}	angles	θ_0	K_{angle}	exclusions
MGDG	C4-C6	0.363	38000	C1-C4-C6	63	22	C1-GL2
	C1-C6	0.366	15000	C4-C1-C6	63	17	C4-GL1
	C1-C4	0.326	44000	C6-C1-GL1	139	28	C6-GL1
	C1-GL1	0.360	3000	C1-C6-C4	53	30	
	GL1-GL2	0.414	4000	C4-C1-GL1	133	25	
				C1-GL1-GL2	81	70	
DGDG	C41-C61	0.364	35000	C11-C41-C61	48	30	C12-GL2
	C11-C61	0.274	35000	C61-C11-C62	120	30	
	C11-C41	0.312	16000	C41-C11-C62	156	40	
	C11-C62	0.369	15000	C11-C62-C42	145	25	
	C42-C62	0.315	35000	C11-C62-C12	106	35	
	C12-C62	0.346	25000	C62-C42-C12	65	25	
	C12-C42	0.325	35000	C62-C12-C42	56	35	
	C12-GL1	0.372	3900	C62-C12-GL1	151	30	
	GL1-GL2	0.414	4500	C42-C12-GL1	123	35	
				C12-GL1-GL2	77	40	
SQDG	C6-S6	0.360	25000	S6-C6-C4	126	60	S6-C4
	C4-C6	0.250	33000	S6-C6-C1	75	50	S6-C1
	C1-C6	0.340	35000	C6-C1-GL1	165	30	C1-GL2
	C1-C4	0.290	34000	C4-C1-GL1	124	35	
	C1-GL1	0.370	5600	C1-GL1-GL2	85	60	
	GL1-GL2	0.385	4900				

Table S1. Bonded interaction parameters for the alternative MGDG, SQDG, and DGDG models. Labeling nomenclature is indicated in figures S1 and S2. Bonds with force constants larger than 25,000 are treated as constraints in practice.

Lipid	state	APL	Thickness	T_M
MGDG	gel	0.470	4.8	306
	liquid	0.567	4.3	310
DGDG	gel	0.520	4.6	290
	liquid	0.590	4.2	295
SQDG	gel	0.479	4.8	328
	liquid	0.564	4.3	333

Table S2. Properties of glycolipid membranes close to the main phase transition temperature Tm, obtained with the alternative CG model. Area per lipid (APL) calculated as the average box size in the xy-plane divided by the number of lipids per monolayer. Membrane thickness was determined from the maxima of the electron density profiles of the system. The estimated value of Tm is in between the indicated temperatures for which the structural properties of the gel and liquid phase were obtained.

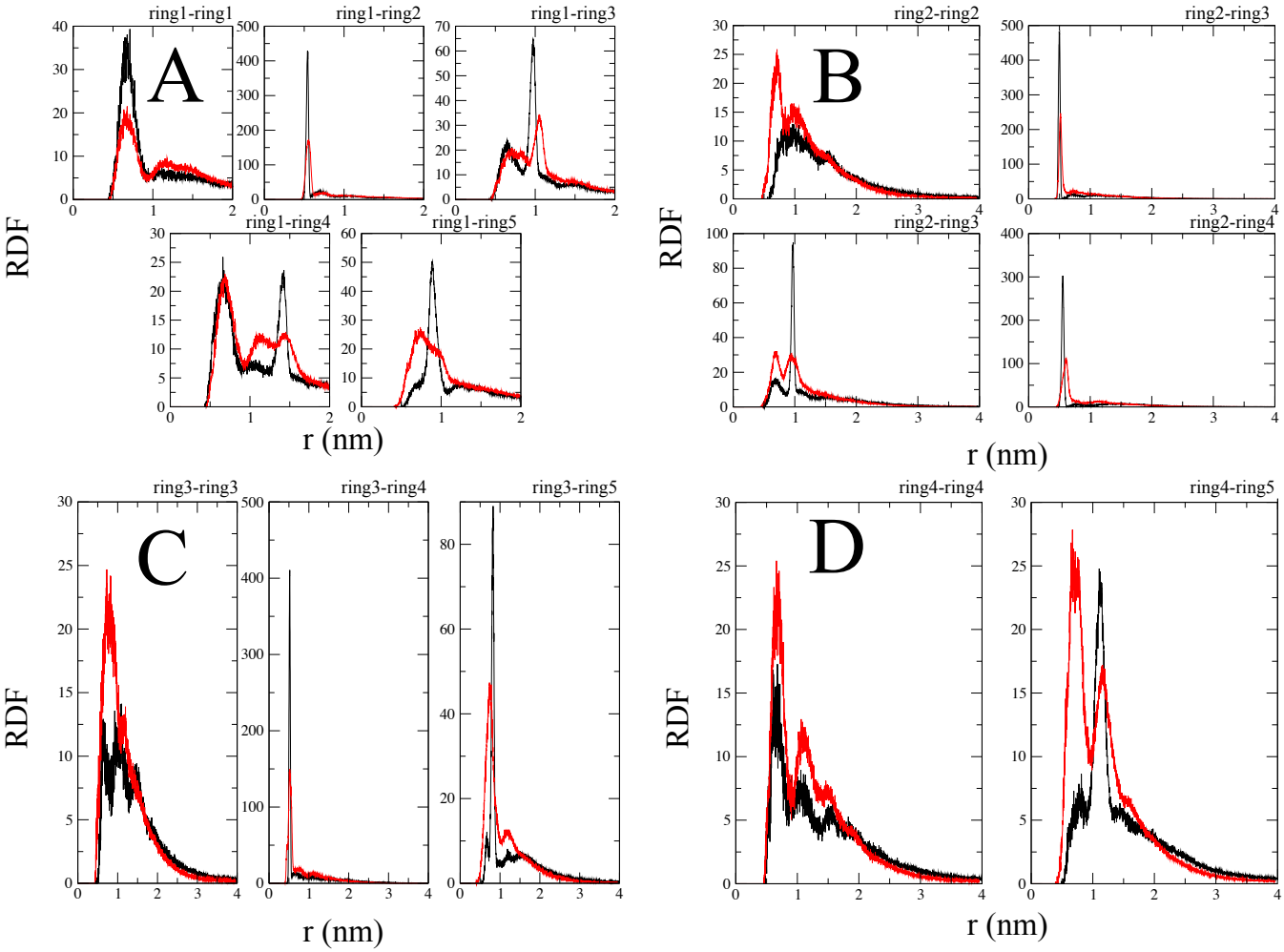

Figure S3. Complementary RDFs of GM1. RDFs were calculated for individual sugar rings of GM1 as described in the main manuscript. RDFs are depicted at AA (black lines) and CG (red lines) resolution.

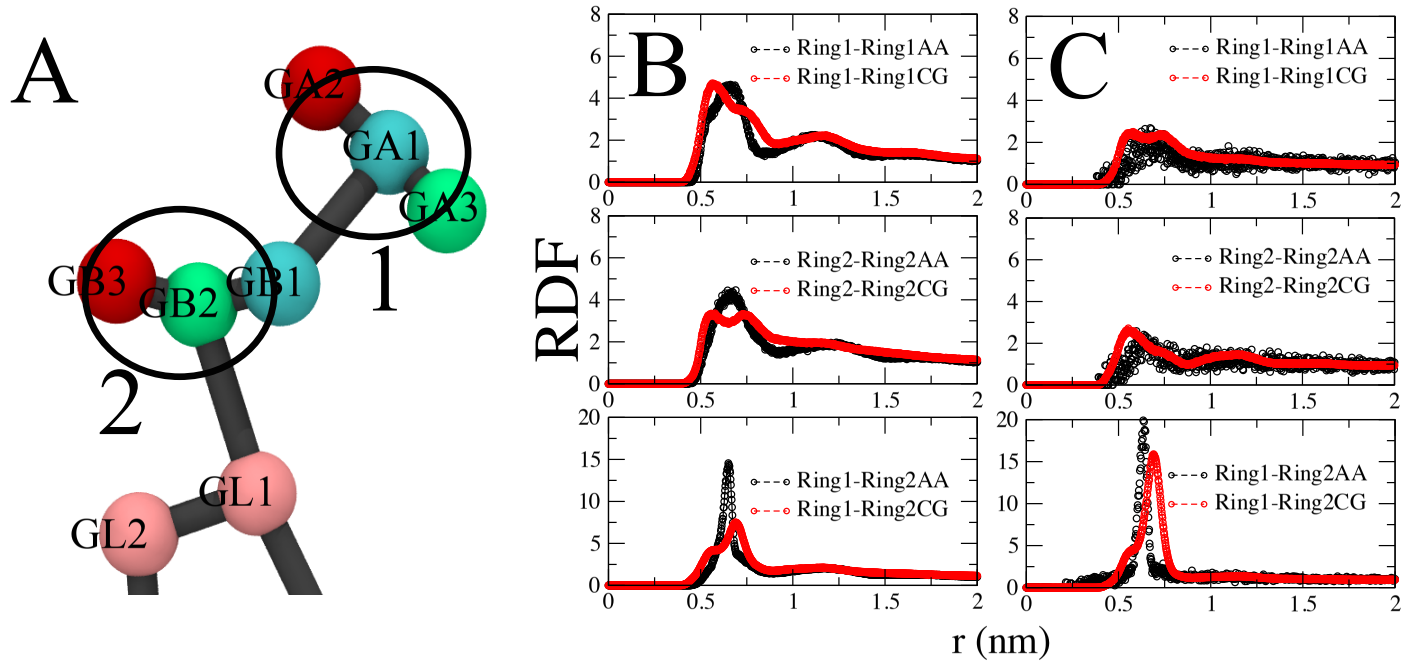

Figure S4. RDFs of independent sugar rings of DGDG. (A) Visual description of the DGDG head group at the CG level, with the topological definition of ring 1 and 2. (B) RDFs of the DGDG head group in a fluid membrane. (C) RDFs of the DGDG head group in aqueous solution. RDFs were calculated for both AA (black line) and CG (red line) resolution.