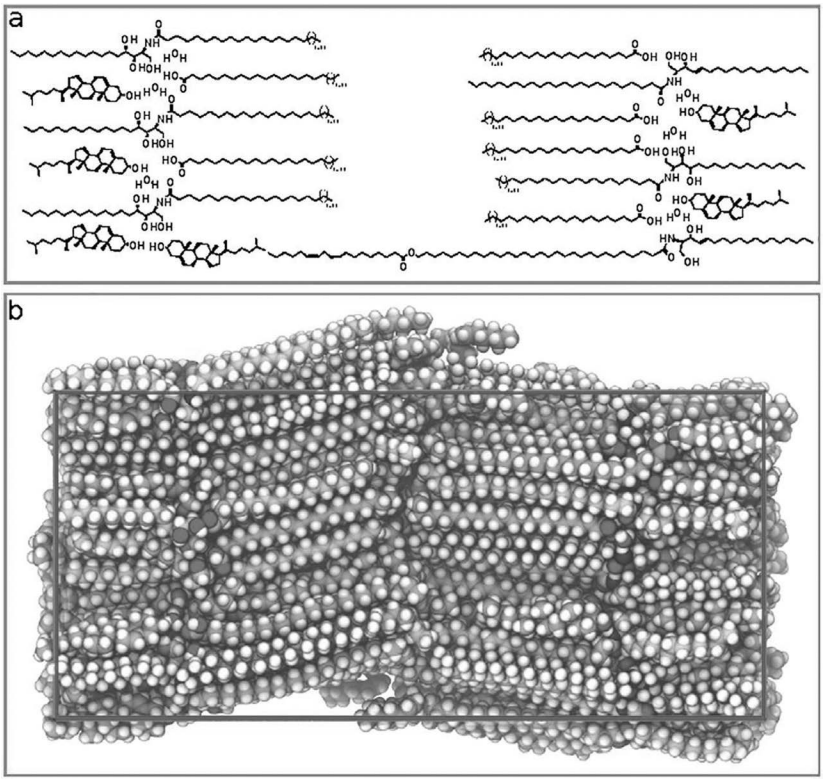

FIGURE 1.2 The molecular organization of the skin's lipid structure. The optimized MD model system for the skin's lipid structure validated against CEMOVIS data from skin. (a) A schematic drawing of the model system, where the ceramide fatty acid and free fatty acid chain lengths are just included as a range. The basic lipid arrangement is that of stacked bilayers of fully extended ceramides with cholesterol largely (about 75%) associated with the ceramide sphingoid moiety. (b) The model system after the MD simulation production phase.

the ceramide sphingoid moiety and all the free fatty acids associated with the ceramide fatty acid moiety. A restricted number of water molecules are associated with the lipid headgroups (about one water per ceramide headgroup), and the lipid structure also contains some acyl-ceramides (about 5 mol%) (Lundborg et al., 2018a) (Figure 1.2a).

Recently, a thermodynamically equilibrated atomistic MD model of the skin's lipid structure has been constructed (Figure 1.2b) and validated against high-resolution CEMOVIS data from near-native skin (Lundborg et al., 2018a) (Figure 1.3). The dynamics of the skin lipid molecules differ along the chains. The mobility is highest at the interface between opposing ceramide fatty acid and free fatty acid chains. Ester-bound linoleic acid chains of the acyl-ceramides accumulate at this interface, contributing, together with the skin lipids' broad ceramide fatty acid and free fatty acid chain length distribution, to the higher lipid chain mobility in this interface region (Lundborg et al., 2018a).

1.4 SKIN BARRIER PERMEABILITY AND THERMOTROPIC BEHAVIOR

The new MD model of the skin's lipid structure has permeability properties, as well as a thermotropic behavior, compatible with that of human skin (Lundborg et al., 2018a,b). Water has a large and complex effect on the skin's permeability depending on the permeant (water or other compound),