



FIGURE 1.4 Experimental procedure for the analysis of cryo-EM (CEMOVIS) data using MD simulation and EM simulation. Outline of the general procedure for analyzing the structure and composition of the system by comparing simulated EM images generated from candidate atomic models after MD simulation with experimental cryo-EM images obtained from near-native human skin, using an iterative approach. The candidate model system is modified (regarding relative ceramide, free fatty acid, and cholesterol concentrations; cholesterol distribution; acyl-ceramide content; and amount of water in the membrane) until good agreement with experimental data is achieved. (Adapted from Lundborg et al., 2018a with permission.)