Fig. 4. The lowest energy conformations of the FCC homopolymers of length 12, 24, and 32 amino acids (the last of these is shown from the side and above) found by the algorithms we tested; the corresponding energies are: \(-39\) for \(N = 12\) (short-range energy = \(-28\), long-range energy = \(-11\)), \(-109\) for \(N = 24\) (short-range energy = \(-68\), long-range energy = \(-41\)) and \(-161\) for \(N = 32\) (short-range energy = \(-112\), long-range energy = \(-49\)). These conformations are specified in detail in the supplementary material.

Fig. 5. Distribution of run-times required by MC, REMC, PHAT and BINMC to reach sub-optimal conformations with energy \(-158\) for the homopolymer of length 32 (part a) \(-370\) for the homopolymer of length 64 (part b), based on 100 independent runs on our reference machine, each of which reached the target energy value. We fitted the run-time distribution (RTD) of BINMC for the homopolymer of length 64 with exponential distribution, to illustrate that the respective RTD is approximately exponential. (The same holds for all other RTDs shown in these plots.)