r.m.s.d.'s between MD average structures and the starting X-ray structures correlate with atomic resolution.

The r.m.s.d.'s between main-chain atoms in the starting X-ray structures and simulation snapshots as a function of time are presented in Fig. 20.2.8.2. The 1.1 Å resolution structure has the most stable trajectory during the 500 ps trajectory, with an average r.m.s. value of 1.01 (9) Å. The 1.7 Å resolution structure has an r.m.s. value of 0.98 (22) Å. In this simulation, the r.m.s.d.'s fluctuate more widely from the average value, with small differences in the first 200 ps, larger ones between 200 and 400 ps, and again smaller ones in the last 100 ps. For the 2.7 Å resolution structure, the average over the simulation is 1.28 (21) Å. From the results presented here, it is concluded that the higher-resolution structures are more stable during MD simulations and have a shorter equilibration period (50 ps for 1.1 Å resolution and over 300 ps for 2.7 Å resolution). This conclusion is consistent with larger errors in the atomic coordinates of X-ray structures determined from lower-resolution data.

Acknowledgements

This work was supported by grants to CBP from the NIH (R01-GM39478, AI39639). CBP was supported by a Research Career Development Award from the NIH (K04-GM00661) and VMD is a DOE/SLOAN Postdoctoral Fellow in computational biology. The computing facilities shared by the Structural Biology group were supported by grants from the Lucille P. Markey Foundation and the Purdue University Academic Reinvestment Program.

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