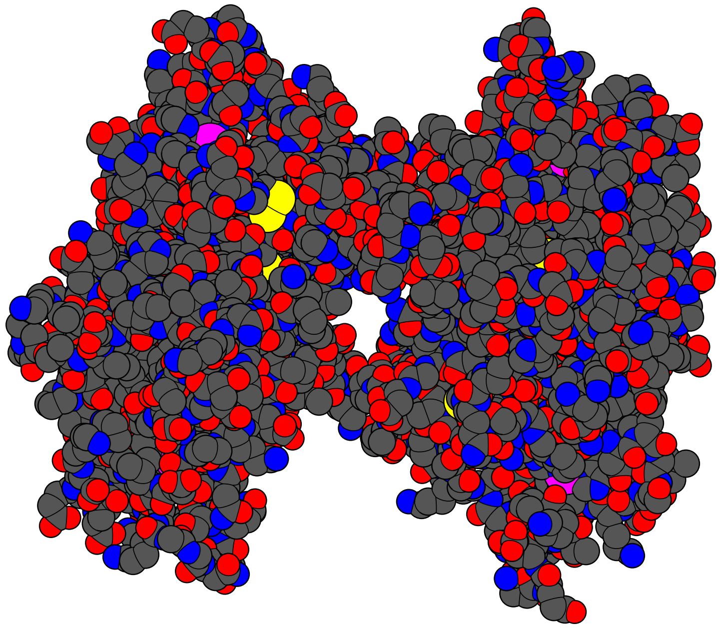

Figure 3: Test molecule SOD (SuperOxide Dismutase) with 4392 atoms.

Hence, by volume consideration, the total number of balls that are completely contained in B cannot exceed

$$\frac{(r_i + 2r_{\max})^3}{(\frac{\rho}{2} \cdot r_{\min})^3} \le \frac{(3r_{\max})^3}{(\frac{\rho}{2} \cdot r_{\min})^3} \le 216 \cdot (\frac{k}{\rho})^3.$$

Part (ii) follows from Part (i) because Part (i) implies that the number of features involving B_i on the union boundary is bounded by a constant. Indeed, if the balls are in general position then a feature involving a ball B_i is either a face on the boundary of B_i, or an intersection arc of B_i with another ball, or an intersection point of B_i with two other balls. All these features belong to the two-dimensional subdivision (or *arrangement*) formed on the boundary of B_i by a constant number of circles, each being the intersection of B_i with another ball. The complexity of this arrangement is evidently bounded by a constant. Thus, the overall complexity of the union boundary is $O(n)$. □

The following table gives the values of k, ρ and the maximal and average number of balls intersecting a single ball for our five example molecules (Figures 1 through 3).

molecule	k	ρ	max	aver.
caffeine	2.17	0.71	10	4.5
acetyl	3.11	0.67	16	5.4
crambin	1.64	0.78	10	5.5
felix	1.64	0.81	9	4.9
SOD	1.95	0.76	16	5.5

As can be seen k is small and ρ is large as required, resulting in a small number of intersections per ball (being much smaller than the worst-case bound of $216(k/\rho)^3$).

We now turn to discuss the subdivision of three-dimensional space induced by a collection of spheres: the *arrangement* of the spheres. The study of arrangements plays a fundamental role in geometric computing, and arrangements arise in the design and analysis of algorithms for a large variety of applications. We denote the arrangement of the spheres in M by $\mathcal{A}(M)$, that is, $\mathcal{A}(M)$ is the subdivision of 3-space into cells of dimensions $0, 1, 2$ and 3, induced by the spheres in M (see [4]). A 0-dimensional cell (a vertex) of the