

cal axis direction would then be approximately 75 Å, which is very close to what is seen in the nucleosome structures. Furthermore, the octamer of Burlingame then forms ramp and groove-like regions precisely where they are seen in our own nucleosome structure. We suggest that Burlingame *et al.* seriously reconsider the model DNA placement on a condensed histone octamer structure.

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Instead of using a heavy atom derivative to phase their 15 Å data set, Uberbacher and Bunick (1) used molecular replacement and model building to obtain a structure for the nucleosome core particle. In this process they used the structure of Richmond *et al.* (2) as their starting point. Their structure is dominated by the features of their starting model, since this is the expected result of the molecular replacement operation. Continuing their model building, they have now drawn lines representing DNA on our photographs (3), thus developing an additional model for the structure of the core particle. They appear to have generated this model in order to compact our octamer structure and force it to resemble the model of Richmond *et al.* We do not feel the need to do so and our reasons are presented in our reply to Klug *et al.* (4).

The model proposed by Uberbacher and Bunick requires that the length of the histone octamer be condensed to 75 Å. The so-compacted structure, which represents an averaging of the length of the structure of Richmond *et al.* with ours, does not fit parameters imposed by diffraction data. It is well known that the diffraction pattern of chromatin consists of the first- and higher orders from a Bragg spacing of 110 Å, that is, 1/110, 1/55, 1/37, 1/27 (5). Our model-built nucleosome is roughly spherical and is 110 Å in diameter. The pitch of the DNA is about 37 Å, and the tripartite protein core is roughly divided into three 37-Å long pieces. Thus the first-order reflections from the DNA superhelix and from the internal arrangement of the protein would superimpose on the third-order from the whole particle. Both our model and that of Richmond *et al.* are consistent with the above criteria, but the model presented by Uberbacher and Bunick would give additional reflections, which are not observed. Averaging two differing structures does not yield the correct one.

In the modeling studies of Uberbacher and Bunick, the value initially assumed for the length of the octamer was 50 Å, and no new value was reported as a result of their procedures [reference 1 in (1)]. The dimensions that they cite now for the structure in Fig. 1 (1) differ from those that can be obtained by measuring directly the model shown there, when the dimensions of our balsa wood model are used as a scale. The superhelical radius is 48 Å (not 43 Å), the superhelical pitch is 37 Å (not 28 Å), and the length of the particle parallel to the superhelical axis and measured only to the outermost edges of the DNA is 94 Å (not 75 Å). Furthermore, direct inspection of our three-dimensional octamer structure reveals that there is some room for *small-scale* closure of the dimer-tetramer channels at the *front* if the dimer is allowed to pivot about the dimer-tetramer contact point at the back. However, there is no

space available to permit the dimer to shift inward along the entire channel, and there is no evidence suggesting that the dimensions of the octamer change drastically when it associates with DNA (4).

We have already stated that we have attempted several alternate placements of the DNA around the histone octamer (3, p. 551). We have published our preferred orientation in which the DNA "follows the path dictated by these grooves and ridges" (3, p. 550), not just the grooves. We found two other interesting orientations. In one (left-tilt), the DNA path is tilted 30 to 45 degrees to the left (similar to theirs) of the path it occupies in our preferred orientation, while in the other (right-tilt) the DNA path is tilted about 45 degrees to the right. In the right-tilt model the DNA rides on the front of the long "propeller" of the H3. The histone octamer remains 110 Å long in all three models, each of which has its own probability of existing *in vivo*. However, in the absence of direct information on the DNA location, we did not present these models to avoid contributing to excessive speculations.

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Crystallographic Structure of the Octamer Histone Core of the Nucleosome

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