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Structural flexibility revealed by ultra-high resolution data

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Not many macromolecular crystals diffract X-rays to ultra-high resolution, defined usually as higher than 0.8 Å, and in the Protein Data Bank there are currently 43 such submissions. These structures range in size from antibiotics of about a hundred atoms to proteins with more than 3,000 independent atoms in the asymmetric unit of the crystal cell. The unprecedented data resolution reveals a great wealth of structural details, which cannot be visualized by analyses at lower resolution. The accuracy of the refined stereochemical and geometrical parameters is then comparable with values typical for small-molecular crystallography and exceeds the accuracy of the library of the standard restraint target values, routinely used in refinement of proteins and nucleotides. Somewhat unexpectedly, the very high resolution diffraction does not necessarily relates to extreme stability of the crystallized molecules, so that the obtained electron density maps reveal significant parts of the atomic models existing in multiple conformations, slightly differing from each other. For example, about 1/3 of the protein chain in the 0.65 Å structure of lysozyme [1] and majority of phosphate groups in the 0.75 Å structure of Z-DNA dodecamer [2] could be modeled in double conformations.

[1] *Wang, J., Dauter, M., Alkire, R., Joachimiak, A., Dauter, Z. Acta Cryst. D63, 1254–1268 (2007).,* ***[2]*** *Luo, Z., Dauter, M., Dauter, Z. Acta Cryst. D70, submitted.*

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