Poster Presentations

[MS5-P22] Phasing Z-DNA Dodecamer Using Anomalous Signal of Phosphorus

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The amount of phosphorus in all nucleic acid is almost constant. At wavelength 1.54Å, phosphorus has an *f"* value of 0.433 and sulfur 0.556 electrons. The expected value of $<\Delta F_{anom}/F>$ for data collection from DNA crystals at Cuká wavelength is about 2.0%, significantly higher than the signal expected from sulfur in protein. Using anomalous signal of phosphorus to phase the crystal structure of hexamer duplex $d(CGCGCG)_2$ has been proved to be successful [1]. Due to the weak anomalous signal provided by phosphorus in nucleic acids, more trials are needed to test the applicability of this approach. Here, a dodecamer duplex $d(CGCGCGCGCGCG)_2$ containing 22 phosphates in the molecule was crystallized, and diffraction data with synchrotron radiation of wavelength 1.54Å were collected. In addition, atomic resolution diffraction data were also collected at wavelength of 0.62 Å. The dodecamer duplex $d(CGCGCGCGCGCG)_2$ was crystallized using Nucleic Acid Mini Screen Kit from Hampton Research. Two data sets were measured from the same crystal. The first with wavelength 1.54 Å to a resolution of 1.67 Å, and the second with wavelength 0.62 Å to a resolution of 0.75 Å. Diffraction data were processed using *HKL*2000 [2], with space group *C*2 and cell unit a=48.5, b=19.5, c=31.2, β=116.4, which is different than the typical Z-DNA space groups $P2_12_12_1$ or $P6_5$. *SHELXD* [3] was used to find the phosphorus sites, providing 11 unique P atoms with occupancy >0.32. *SHELXE* [3] was used for density modification with the ultrahigh- resolution native data set. The density map clearly revealed aromatic rings of nucleotides stacked layer by layer. The crystal structure was refined by *SHELXL* [3]. There is only one helix chain in an asymmetric unit of the dodecamer crystal structure, while the other chain can be generated by a simple rotation along the crystallographic 2-fold axis. There are double conformations of phosphodiester backbone at certain sites of the dodecamer crystal structure, which can be assigned to Z_I or Z_{II} conformation. Although the crystal packing of the dodecamer duplex is very similar to the hexamer duplex from the top view of the duplex, the orientation of helices is quite different. In conclusion, a new successful case of using anomalous signal of phosphorus to phase DNA structure is presented. Possibility of multiple conformations and differences in packing orientation should be considered during further studies of the structures of nucleic acids.

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