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Data article

Diffraction anisotropy falloff in the direction of the detergent belt for two centered monoclinic crystals of OmpF

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ABSTRACT

This data article describes the anisotropy of diffraction observed for the centered monoclinic crystals of OmpF reported in "Two different centered monoclinic crystals of the *E. coli* outer-membrane protein OmpF originate from the same building block (Chaptal et al., 2016 [1])". The datasets intensity falloff as a function of resolution are provided along with reflections along the (h,l) and (k,l) planes. A comparison with the crystal packing in the real cell is also provided, with the correspondence to the reciprocal vectors. These data can be retrieved from the Protein Data Bank under accession codes PDB: 4jfb and PDB: 4d5u.

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Specifications Table

Subject area	*Biology*
More specific subject area	*Crystallography*
Type of data	*Figure*
How data was acquired	*X-ray diffraction of crystals.*
Data format	*Analyzed*
Experimental factors	*Comparison of the direction of diffraction anisotropy in reciprocal space and lack of protein:protein contact in real space.*
Experimental features	*The reflection files were subjected to anisotropy analysis using the UCLA anisotropy server, and simulated diffraction images along the h=0 and k=0 were generated in the Phenix package.*
Data source location	*Data for the crystal in C2 with tNCS were collected at the ESRF, and data in I2 were collected at ALBA synchrotrons, respectively.*
Data accessibility	*Data is within this article. Protein Data Bank under accession codes PDB: 4jfb and PDB: 4d5u.*

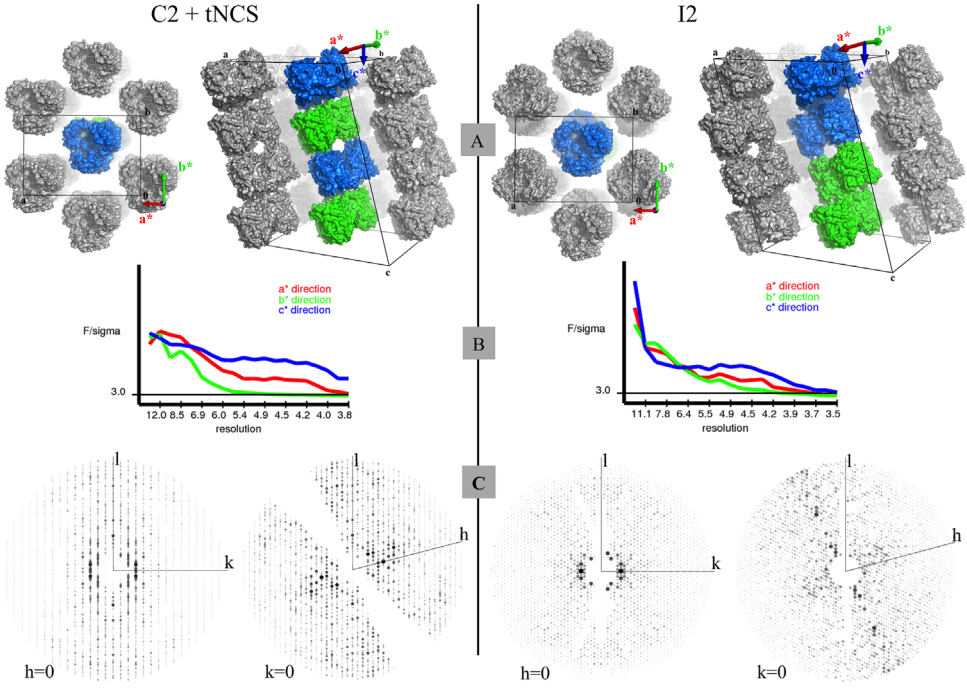

Fig. 1. Diffraction anisotropy and crystal packing of OmpF centered monoclinic crystals. Left side: C2 with tNCS; right side: I2. **A/** The real cell is drawn in black with the origin (**O**) and the letters (**a**, **b**, **c**) symbolizing the real vectors. The reciprocal cell is outlined on the side, with vectors **a***, **b*** and **c*** colored in red, green and blue, respectively, to mimic panel B. The reciprocal cell values have been determined using the online server, http://www.ruppweb.org/new_comp/reciprocal_cell.htm, and their size have been multiplied by 5000 to be able to visualize them next to the real cell. To picture crystal packing, top and side views of the two cells display OmpF in surface, with the asymmetric unit in blue, one symmetric in green and the other symmetric molecules in grey (coloring scheme similar to [1]). For the side view, the front symmetric molecules have been removed for clarity. **B/** diffraction anisotropy analysis of the whole dataset as given by the UCLA anisotropy server (http://services.mbi.ucla.edu/anisoscale/). **C/** projections of the reciprocal lattice planes $h=0$ and $k=0$ to visualize the relative diffraction strength along the three dimensions. Figures were created with Pymol [6].