Data in Brief 11 (2017) 552–556

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Crystallographic anomalous diffraction data for the experimental phasing of two myelin proteins, gliomedin and periaxin

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ARTICLE INFO

Article history:
Received 22 November 2016
Received in revised form
11 January 2017
Accepted 27 February 2017
Available online 6 March 2017

Keywords:
Crystallography
Protein
Anomalous signal
Experimental phasing
Synchrotron

ABSTRACT

We present datasets that can be used for the experimental phasing of crystal structures of two myelin proteins. The structures were recently described in the articles "Periaxin and AHNAK nucleoprotein 2 form intertwined homodimers through domain swapping" (H. Han, P. Kursula, 2014) [1] and "The olfactomedin domain from gliomedin is a β-propeller with unique structural properties" (H. Han, P. Kursula, 2015) [2]. Crystals of periaxin were derivatized with tungsten and xenon prior to data collection, and diffraction data for these crystals are reported at 3 and 1 wavelengths, respectively. Crystallographic data for two different pressurizing times for xenon are provided. Gliomedin was derivatized with platinum, and data for single-wavelength anomalous dispersion are included. The data can be used to repeat the phasing experiments, to analyze heavy atom binding sites in proteins, as well as to optimize future derivatization experiments of protein crystals with these and other heavy-atom compounds.

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http://dx.doi.org/10.1016/j.dib.2017.02.049

Specifications Table

Subject area	*Biology*
More specific subject area	*Structural biology*
Type of data	*Diffraction datasets, graphs, tables*
How data was acquired	*Synchrotron X-ray data collection*
Data format	*Processed raw anomalous data from diffraction images in ASCII format*
Experimental factors	*Data from protein crystals subjected to heavy atom derivatization*
Experimental features	*Crystals of periaxin and gliomedin were derivatized with heavy atoms, and anomalous diffraction datasets were collected using synchrotron radiation.*
Data source location	*BESSY, Berlin, Germany*
Data accessibility	*The derivative data are presented in this article and available as* Supplementary material.

Value of the data

- Structure solution for periaxin and gliomedin can be reproduced.
- Heavy atom binding to proteins can be understood.
- Derivatization conditions for protein crystals can be optimized.
- Different experimental phasing approaches can be employed.
- The strength of the anomalous signal and diffraction intensity can be studied.

1. Data

We recently solved the crystal structures of periaxin and gliomedin [1,2], and the native crystal data were submitted to the PDB. Here, we include all original unpublished native and derivative datasets used for experimental phasing of the crystal structures, as well as Supplementary datasets with different levels of anomalous signal. The crystallographic data are in Supplementary material, in the output format of the XDS data processing program [3], as this data format allows a variety of further workflows in different software, either directly or after format conversion. In addition, a table of all data processing statistics is given, as are graphs indicating the level and quality of the anomalous signal and diffraction intensity in the different datasets.

2. Experimental design, materials, and methods

The preparation of recombinant protein and crystallization for the periaxin PDZ (post-synaptic density-95, discs large, zona occludens-1)-like domain and the gliomedin olfactomedin (OLF) domain have been described [4,5]. Crystals of the periaxin PDZ-like domain were obtained in 30% polyethylene glycol (PEG) 2000 monomethyl ether, 0.1 M KBr at +4 °C, and tungsten derivatization was completed by soaking the crystals in 5 mM $(NH_4)_2WS_4$ for 2 days, while Xe-derivatized crystals were prepared at the beamline, by incubating fresh crystals in a Xe chamber at 200 psi for either 2 or 8 min.