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Data Article

Data on crystal organization in the structure of the Fab fragment from the NIST reference antibody, RM 8671

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ABSTRACT

The reported data describe the crystallization, crystal packing, structure determination and twinning of the unliganded Fab (antigen-binding fragment) from the NISTmAb (standard reference material 8671). The raw atomic coordinates are available as Protein Data Bank structure 5K8A and biological aspects are described in the article, (Karageorgos et al., 2017) [1]. Crystal data show that the packing is unique, and show the basis for the crystal's twinned growth. Twinning is a common and often serious problem in protein structure determination by x-ray crystallography [2]. In the present case the twinning is due to a small deviation (about 0.3 nm) from 4-fold symmetry in the primary intermolecular interface. The deviation produces pseudosymmetry, generating slightly different conformations of the protein, and alternating strong and weak forms of key packing interfaces throughout the lattice.

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Specifications Table

Subject area	*Biology, Molecular Biology*
More specific subject area	*Protein crystallography, Structural immunology*
Type of data	*Tables, Molecular graphics figures, Structural measurements*
How data was acquired	*Crystallography and molecular structure measurement*
Data format	*Analyzed*
Experimental factors	*Water was removed from the PDB file. Contacts are based on PDBePISA.*
Experimental features	*Packing geometry was analyzed to determine cause of crystal twinning*
Data source location	*Crystal diffraction was measured at the Advanced Photon Sources (aps.anl.gov). All other protocols and analysis were completed at NIST/IBBR*
Data accessibility	*Structural data is at* www.rcsb.org/pdb/explore.do?structureId = 5K8A

Value of the data

- These data describe the molecular packing in the atomic structure of a reference antibody Fab fragment, with implications for crystal growth and structure determination.
- The structure includes the complicating features of twinning and pseudosymmetry; these are described graphically and measured.
- The data provide evidence for the structural basis of the observed twinning.
- Although the described structure and packing are unique, twinning is a common problem in protein structure determination, and the described method/data provide an example that applies broadly to a large class of protein crystal structures.

1. Data

Table 1 gives primary crystal data, Fig. 1 shows the crystals, and Fig. 2 shows the structural variation in the four unique molecules in protein data bank (PDB) structure 5K8A [1], which is the 50 kDa

Table 1
Primary crystallographic data for apo NISTmAb Fab structure (PDB:5k8a).

Diffraction	
Space group	I222
a, *b*, *c* (nm)	14.916, 14.920, 19.503
Resolution range (nm)	3.000 – 0.200 (0.205 – 0.200)
R_{merge}[a]	0.083 (0.817)
Resolution (nm) at which $<I/\sigma(I)> = 2$	0.213
Completeness (%)	99.7 (97.6)
Redundancy	5.9 (4.5)
Refinement	
Nonhydrogen protein atoms	13,436
Water molecules	372
R_{work}/R_{free}	0.166/0.239
Overall Mean *B*-value (nm^2)	0.449
Bond lengths rmsd from ideal (nm)	0.0008
Bond angles rmsd from ideal (degrees)	1.35
Residues refined	1742 (4 independent copies of Fab)

Data collection statistics for the highest resolution shell are given in parentheses.

[a] $R\text{merge} = \Sigma\, |I - <I>| \,/\, \Sigma\, I$ where $<I>$ is the mean of symmetry-related reflection intensities.