02.1-4 THE CRYSTAL STRUCTURE OF FAB NQ10.
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Fab NQ10, derived from a murine monoclonal anti-phenyloxazolone antibody crystallizes in the space group C2 with a = 119.2, b = 78.3, c = 86.0 Å, β = 137.5°. The V_H gene encoding most of the V_H domain of this antibody is closely related to the corresponding gene of the anti-lysozyme D1.3. However, the light polypeptide chain of NQ10 is unrelated to that of D1.3.

Native Fab NQ10 X-ray intensities were measured on a four circle diffractometer to 4.5 Å resolution. Two heavy atom derivatives were obtained using UO_2-acetate at different concentrations. An electron density map at 6 Å resolution clearly revealed the molecular boundaries. Using a rigid body refinement program and the three-dimensional structure of Fab D1.3, a model was fitted to the electron density map showing the traces of the light and heavy chains. The model was refined to 4.5 Å resolution. Measurement of intensities to higher resolution and further refinement of the model are currently under way. The latest progress in the structure determination will be reviewed.

02.1-5 PRONOUNCED EFFECT OF THE SOLVENT OF CRYSTALLIZATION ON THE STRUCTURE OF A MULTI-DOMAIN PROTEIN.
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Radically different variable domain interactions were observed in antibody light-chain dimers crystallized from either distilled water or from 1.5 M ammonium sulfate. Light chains are characterized by an amino-terminal variable domain and a carboxyl-terminal constant domain linked by an extended peptide. We had previously determined the structure of light-chain dimer Loc in a crystal form obtained from ammonium sulfate (C.-Chang, et al., 1985, Biochemistry 24, 4890). The two variable domains form a very unusual antigen binding site consisting of a protrusion with a groove on each side. We now have determined the crystal structure of Loc as crystallized from distilled water. At present, the R = 35% for 3.5 Å data. In this structure, the association of the two variable domains forms a cavity that resembles the "conventional" antigen binding site that was observed in the Mcg protein. The association of the constant domains is very similar in the two crystal forms. Two independent hinge-bending motions are required to convert the structure observed in one crystal form to that observed in the other form. Work supported by the U. S. Department of Energy under contract no. W-31-109-ENG-38.

02.1-6 CRYSTALLIZATION AND CRYSTALLOGRAPHIC STUDY OF PIG LIVER NADH-CYTOCHROME b_5 REDUCTASE.
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NADH-cytochrome b_5 reductase(EC 1.6.2.2) catalyzes to reduce cytochrome b_5 in an electron-transport chain from NADH to a terminal oxidase desaturase in the endoplasmic reticulum. The enzyme is an amphipathic membrane-bound flavoprotein with a single subunit containing one molecule of FAD. The protein molecule consists of a large, hydrophilic catalytic domain and a smaller, hydrophobic membrane-binding domain. We have crystallized the following two forms of this enzyme from pig liver microsomes; the intact molecule(35kDa) solubilized by a detergent (Triton N-101) and the catalytic domain(30kDa) solubilized by a protease(cathepsin D). Crystals have been grown from polyethylene glycol solutions by the vapour diffusion method. The crystals of the intact enzyme are needle-shaped but still too small for X-ray studies(their diameters less than 0.05mm). The crystals of the catalytic domain are large enough(*ca.*0.5×1.0×1.5mm) and belong to the orthorhombic space group $P2_12_12_1$ with unit-cell dimensions of a=87.1, b=73.2, c=49.0 Å. The asymmetric unit contains one protein molecule, the V_M value being 2.6 $Å^3$/Da. X-ray diffraction patterns extend to 2.0 Å resolution. Data collection of native crystals and search for heavy-atom derivatives are currently underway.

02.1-7 CRYSTALLIZATION OF A COPPER CONTAINING NITRITE REDUCTASE
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Two bacteria, "Achromobacter cycloclastes" and Alcaligenes faecalis S-6, contain denitrification pathways in which a small blue copper protein (cupredoxin) transfers electrons to a copper containing nitrite reductase (NIR).(Liu, M.-Y., et al. (1986) J. Bacteriol. 166 604-608; Kakutani T. et al. (1981) J. Biochem. 89 463-472.) The structure of cupredoxin from A. faecalis S-6 is being refined in our lab using data to 2.4Å: the chain tracing (Adman, E.T. et al (1985) Amer. Cryst. Assoc. Abst. Stanford, p.40.; Petratos, K. (1984) PhD thesis, Wayne State Univ.) shows the molecule to be similar to azurin and plastocyanin.
We have obtained small crystals of the cupredoxin from "A. cycloclastes" and data quality crystals of its partner, NIR. NIR is a gray-green protein, a dimer of molecular weight 69kD, (monomer 36.8kD) and three Cu per 69kD. It is crystallized from 32% saturated ammonium sulfate, pH5.0, in 20mM phosphate buffer at 4 °C. The space group, determined from precession photographs, is $P2_13$, a=b=c=98.4 Å. The ratio of crystal volume to molecular weight is 2.16 with one 36.8 kD unit per asymmetric unit (43% solvent).
Preliminary oscillation photographs were taken by Dr. Samar Hasnain and Dr. Yoshinori Satow at the Photon Factory U-14 facility using a crystal .25x.25x.3 mm^3 and highly monochromatized radiation at λ = 1.300±0.002 Å. 150-300 second polaroid exposures show clearly resolved reflections to a d-spacing of at least 1.7Å. Diffraction photographs of crystals soaked in uranyl nitrate or platinum thiocyanate show intensity changes indicative of good derivatives.
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