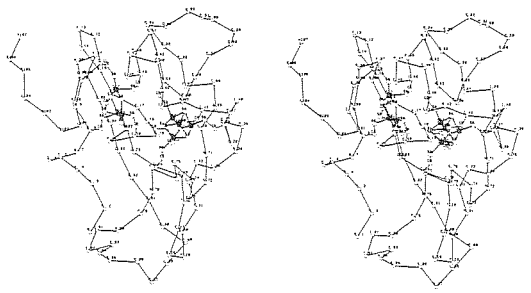
02.X-13 REFINED STRUCTURE OF AZOTOBACTER FERREDOXIN (IRON-SULFUR PROTEIN III) AT 2.0 Å RESOLUTION. By C. D. Stout, D. Ghosh, W. Furey, Jr. and S. O'Donnell, Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260 USA.

The crystal structure of the 7Fe 'ferredoxin' (iron-sulfur protein III) from A. vinelandii has been solved and refined at 2.0 Å resolution. The crystals are tetragonal, $P4_32_12$, a = 55.22, c = 95.20 Å, Z = 8. The polypeptide chain trace was derived from a 3.0 Å MIR map (Ghosh, et al., J. Biol. Chem. 256, in press, 1981). Derivatives were prepared with K_2PtCl_4, $K_2[OsO_2(OH)_4]$ and Na_3RhCl_6; the figure of merit for 3322 reflections is 0.74. Fe atom positions were independently derived from Bijvoet difference Fourier maps at 2.5 Å resolution. The amino-acid sequence (107 residues, MW 12,850 daltons) was determined in collaboration with Dr. J. B. Howard. The protein model was built using the MMS-X graphics system. The structure has been refined by the Hendrickson/Konnert least squares method with programs provided by Dr. W. Furey. R is 0.247 for 856 protein atoms and 327 water molecules for 6249 reflections at 6.0 $\sigma(|F|)$ in the range 10.0-2.0 Å. The rms Δd from ideality is 0.025 Å for 2406 interatomic distances; the average isotropic B is 12.82 $Å^2$.

The molecule contains both low potential [3Fe-3S] and high potential [4Fe-4S] clusters which are separated by 12 Å. The structure consists of an N-terminal core of residues 1-49 which forms the Fe-S sites, and a C-terminal chain of residues 50-107 which enfolds the core. The 4Fe center is coordinated by cysteines 24, 39, 42 and 45; the ligands of the 3Fe center are cysteines 8, 11, 16, 20 and 49 and an uncharacterized small molecule (X), which appears to be water or hydroxyl. The overall protein conformation is suggestive of an enzyme with an active site at the $FeS_2(S_\gamma 16)(X)$ moiety of the [3Fe-3S] cluster. This Fe lies at the base of a cleft and adjacent to a large open loop. Glutamate 18, in the sequence (16-21)CVEVCP, is positioned such that it could interact with Fe or X in the reduced state or during 'catalysis'.



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02.X-14 THE STRUCTURE OF THE INFLUENZA VIRUS HAEMAGGLUTININ GLYCOPROTEIN AT 3 Å RESOLUTION. By I.A. Wilson, J.J. Skehel and D.C. Wiley, Gibbs Laboratory, Harvard University, Cambridge, Mass. U.S.A.

The structure of the haemagglutinin, the major surface antigen of influenza virus has been determined by the method of single isomorphous replacement and non-crystallographic three-fold symmetry averaging (Bricogne, G., Acta Cryst. (1976) A32, 832). The A/Hong Kong/1968 bromelain-released haemagglutinin crystals are $P4_1$, a=163.2 Å, c=177.4 Å with one trimer of 224,640 daltons per asymmetric unit. The molecule contains 19% carbohydrate by weight.

The haemagglutinin is synthesized as a single polypeptide chain with a signal peptide and is subsequently cleavage activated into two chains HA_1 (328 residues) and HA_2 (221 residues). The haemagglutinin binds to host cell sialic acid containing proteins and its cleavage activates membrane fusion activity.

The trimer is an elongated spike projecting some 135 Å from the membrane with a hydrophobic tail embedded in the membrane. The external portion consists of a globular head of mainly antiparellel β-structure on top of a fibrous tail which includes a central triple helical coiled-coil. The carbohydrate is located all along the outside of the molecule (Wilson, I.A., Skehel, J.J. and Wiley, D.C., Nature (1981) 289, 366). Four possible antibody binding sites have been identified on the globular head furthest from the membrane. Amino acid substitutions appear to be required in each location for the production of new epidemic strains between 1968 and 1979. A location for the sialic acid receptor site has been proposed. (Wiley, D.C., Wilson, I.A. and Skehel, J.J., Nature, (1981), 289, 373.)

02.X-15 THE CRYSTAL STRUCTURE OF A PROTEIN PROTEINASE INHIBITOR, PLASMINOSTREPTIN. By Masaaki Matsushima, Osaka Medical College, Takatsuki, Osaka, Japan, Nobuo Kamiya, Faculty of Science, Nagoya University, Nagoya, Japan, and Hiromu Sugino, Central Research Division, Takeda Chem. Ind., Ltd., Yodogawa-ku, Osaka, Japan.

Plasminostreptin was isolated from the culture fluid of *Streptomyces antifibrinolyticus* IFO 13298. It inhibits plasmin, trypsin and subtilisin (Kakinuma *et al.*, J. Biol. Chem. (1978) 253, 1529). It exists as a dimer in solutions. The monomer consists of 109 amino acid residues with two disulfide bonds. The calculated molecular weight is 11402 daltons. The sequence (Sugino *et al.*, J. Biol. Chem. (1978) 253, 1546) is about 70% homologous to that of *Streptomyces* subtilisin inhibitor (SSI) (Ikenaka *et al.*, J. Biochem. (1974) 76, 1191), in spite of the difference in their proteinase-inhibitory spectra. The crystals grown in water at 4°C were transferred into 1.0 M phosphate at pH 6.75. They were orthorhombic, space group $P2_12_12_1$, with the crystal parameters , a = 56.9Å, b = 88.9Å, c = 46.4Å and two molecules in an asymmetric unit. The intensity data were measured with a diffractometer. The heavy atom derivatives were prepared by soaking in 1.0 M phosphate solutions containing 1 mM $HgBr_2$, 1 mM K_2PtCl_4 or 5 mM $KAu(CN)_2$. An electron density map was computed at 2.8Å resolution. The monomer had an anti-parallel β pleated sheet with five strands and two helical structures. One of these helices was on an end of the β sheet and was fixed to the sheet by one of the disulfide bonds. The sheet in the opposite side faced that of the other monomer. These two monomers might be closely related by a local diad. The overall features of the monomer were very similar to those of SSI (Mitsui *et al.*, J. Mol. Biol. (1979) 131, 697). In addition, the quaternary structure of the dimer was also close to that of SSI where the dimer was strictly related to each other by a diad of the crystal symmetry.