02.5-03 CO-CRYSTALLIZATION OF REPRESSOR AND OPERATOR FRAGMENTS FROM BACTERIOPHAGE LAMBDA.
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We have grown crystals that contain an amino-terminal fragment of lambda repressor (residues 1-92) and an eleven-base-pair operator fragment. The operator fragment $\frac{(GTATCACCGCC)}{(CATAGTGGCGG)}$ contains slightly more than half of an operator site, and we believe that it provides a binding site for one amino-terminal fragment. (A repressor dimer binds to each full operator site.) Chemical protection experiments have shown that the amino-terminal fragment of repressor binds specifically to this operator fragment (Alexander Johnson, unpublished).

We have grown two crystal forms that contain the repressor and operator fragments. Hexagonal plates grow in space group $P6_322$ with cell dimensions a=b=67 Å, c=296 Å. Hexagonal pyramids have also been grown. These have cell dimensions of a=b=71 Å, c=281 Å. Both crystal forms diffract to 3-6 Å resolution. (There is anisotropic disorder.) Diffuse scattering at 1/3.4 Å shows that the DNA helices are parallel to the c axis in the hexagonal plates and tipped at about 20° to this axis in the bipyramids. Precession photographs have allowed us to determine the main features of the packing in these co-crystals.

02.5-04 THE X-RAY CRYSTAL STRUCTURE OF SWOLLEN TOMATO BUSHY STUNT VIRUS.
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The structure of 80% of the the protein component of Tomato Bushy Stunt Virus (TBSV) is known at atomic resolution (Harrison et. al., Nature (1978) 276, 368). The virus has been shown by solution scattering to undergo a reversible phase transition whereby the roughly spherical protein shell expands radially by about 20Å. The transition is induced by removal of bound calcium from the native virus and raising the pH above 7.0, and is termed 'swelling'.

The swollen state has been crystalised to give monoclinic crystals containing two particles per unit cell, or half a particle per C2 asymmetric unit. The diffraction limit of the crystals is about 7Å. About 50% of the data to 7.4Å have been collected on 1° oscillation films with a reproducibility R = 0.19 for intensities.

A novel method has been used to phase the observed reflections. A crude model based upon radial expansion of the native structure was refined by an R-factor search and used as a preliminary source of phases (R = 0.52 to 12Å). These were then subjected to refinement by symmetry averaging, using the icosahedral (non-crystallographic) symmetry of the particle, assumed to be valid for the swollen form (R = 0.38 to 12Å). Heavy atom positions for two derivatives were refined using these phases and were found to correspond closely to the native sites, when displaced according to the model. The existence of sensible heavy atom sites with the correct quasi-symmetry is a strong indication that the phases are valid. A more accurate model was constructed to phase the higher resolution terms (R = 0.48 to 8Å) which were once again refined to give a final map of 7.4Å resolution.

The structure shows that the most extensive subunit-subunit contacts are conserved, but that the interfaces containing the calcium binding sites in the native form are disrupted to leave large holes in the particle surface. This may be of significance to the viral assembly mechanism.

02.5-05 THE STRUCTURE OF THE SATELLITE TOBACCO NECROSIS VIRUS.
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The Satellite Tobacco Necrosis Virus (STNV), MW=$1.7 \cdot 10^6$, is a small spherical plant virus with icosahedral symmetry in the protein shell. It requires in vivo co-infection with Tobacco Necrosis Virus for growth. STNV is composed of a coat with 60 identical protein molecules (195 amino acids) and a single-stranded RNA, (about 1,200 nucleotides) known to code for the coat protein.

STNV crystallizes in space group C2 with four particles in the monoclinic cell with a=317.3, b=304.0, c=184.6 and β=94.26°. The crystallographic asymmetric unit contains a complete virus particle. Thus the virus particle is located in a general position in the unit cell, and the crystallographic symmetry does not exclude a determination of even the nucleic acid structure.

2.5 Å native data, 4.0 Å iodine and 2.8 Å platinum chloride derivative data have been collected using oscillation camera technique. The native data set consists of 500 000 measured independent reflexions.

The utilization of the 60-fold non-crystallographic symmetry requires an accurate determination of particle orientation parameters. This has been achived using 1) the rotation function and 2) an icosahedrally constrained heavy atom parameter refinement. Density averaging techniques employing the 60-fold structural redundancy have been used for phase refinement.

REFERENCE:
Unge, T. et al.: Nature 285, 373 (1980); Satellite tobacco necrosis virus structure at 4.0 Å resolution.

02.5-06 CRYSTALLIZATION OF COWPEA CHLOROTIC MOTTLE VIRUS AND BELLADONNA MOTTLE VIRUS.
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Cowpea Chlorotic Mottle Virus belongs to the brome mosaic virus group of the small spherical plant viruses. It contains 180 protein subunits, which are arranged on a T = 3 icosahedral surface lattice. The virus crystallizes in orthorhombic space group $P2_12_12$ (a = 394 Å, b = 382 Å, and c = 397 Å). The unit cell contains four virus particles while the crystallographic asymmetric unit consists of one complete virion. X-ray diffraction data from the crystals extend to nearly 3.0 Å resolution.

Belladonna Mottle Virus belongs to the turnip yellows mosaic virus group of the small spherical plant viruses. It contains 180 protein subunits, which are arranged in a T = 3 icosahedral surface lattice. The top and bottom viral components crystallize isomorphously in hexagonal space group R3 (a = b = 296 Å, c = 729 Å). The unit cell contains three virus particles while the crystallographic asymmetric unit consists of only one-third of a particle. X-ray diffraction data from the crystals extend to at least 3.0 Å resolution.