

in diameter) RNA viruses that have an icosahedrally systematic capsid. This capsid contains 60 copies of each of four coat proteins VP1, VP2, VP3, and VP4. Several structures of picornaviruses have been determined to date, however, no three-dimensional structure is currently available for CVB1. We report here the crystallization, X-ray diffraction analysis, and structure determination of CVB1 complexed to a potent antiviral agent.

Crystals of CVB1 complexed to an antiviral agent in the SCH 47802 series were grown in the presence of Li_2SO_4 and PEG using a modification of the vapor diffusion technique. Small triangular blocks appear in 2-5 days, the largest measuring $0.2 \times 0.2 \times 0.3$ mm. These crystals diffract X-rays to at least 2.6 \AA resolution at CHESS. Data analysis indicates that these crystals belong to space group C222₁ with cell dimensions of $a=345.7$, $b=497.2.4$, and $c=485.9 \text{ \AA}$, and $\alpha=\beta=\gamma=90^\circ$. A dataset was collected at the CHESS F1 station that is 50% complete to 3.0 \AA resolution with a R_{merge} of 10.6%.

Molecular replacement was used to solve the structure using a starting model of coxsackievirus B3. Rotation and translation functions indicate that the particle is rotated 54.8° around the y-axis relative to a standard icosahedral orientation and that the position of the particle center is at $y=0.19$. After the molecular replacement solution was determined, thirty-fold non-crystallographic symmetry averaging was used to improve the electron density and the phases. Electron density consistent with bound antiviral agent is present in the drug binding pocket. Details of the interactions between the antiviral agent and the virus will be presented, as well as a comparison between CVB1 and other picornaviruses.

PS04.09.10 CRYSTALLIZATION OF EIAV p26. Zhongmin Jin^{1,3}, Ashley J. Birkett², Ling Jin², Darrell L. Peterson², Catherine L. Lawson¹. ¹Biology Department, Brookhaven National Laboratory, Upton, NY 11973; ²Department of Biochemistry and Molecular Biophysics, Virginia Commonwealth University, Richmond, VA 23298; ³Department of Physics, State University of New York at Stony Brook, Stony Brook, NY 11790, USA

We report here the crystallization of the p26 core protein from equine infectious anaemia virus (EIAV), a retrovirus of the *Lentiviridae* family. EIAV is responsible for causing a chronic, debilitating disease in horses. Infection has been reported worldwide and EIAV is recognized as a livestock pathogen of significant economic importance to the horse industry. There is significant homology between the non-human *lentiviruses* and HIV-1. The structural study of EIAV gag/core protein will help in understanding the structure of HIV core protein, and in evaluating methods of effective treatment and control of viral infection.

Crystals were grown at room temperature by vapor diffusion with 0.1M Citrate buffer and 10% PEG3300, 15% isopropanol, at pH 6.5. They belong to the space group P6₁22 (or P6₅22) with $a = b = 101 \text{ \AA}$ and $c = 158 \text{ \AA}$. A complete native data set to 3.6 \AA ($R_{\text{sym}} = 11 \%$) has been collected at beamline X12C of National Synchrotron Light Source at Brookhaven National Laboratory. We expect to obtain a higher resolution native, since diffraction from one crystal frozen in liquid propane was observed to 2.8 \AA .

The crystal may contain one or two p26 protomers per asymmetric unit. The space group symmetry and cell dimensions suggest that the packing of p26 protomers may be similar to packing of HIV-1 p24 protein in 100 \AA diameter fibers (Ehrlich et al, 1992). EIAV p26 and HIV-1 p24 have 55% sequence homology and 30% sequence identity.

PS04.09.11 INTERACTION OF INTERCELLULAR ADHESION MOLECULE-1 (ICAM-1) AND HUMAN RHINOVIRUS (HRV) AND THE ROLE OF CHARGE. Prasanna R. Kolatkar, Jordi Bella, Wai-ming Lee*, Roland Rueckert* and Michael G. Rossmann, Department of Biological Sciences, Purdue University, W. Lafayette, IN 47906 *Institute of Molecular Virology, University of Wisconsin, Madison, WI 53706.

Intercellular Adhesion Molecule-1 (ICAM-1) is the receptor used by the majority of human rhinoviruses (HRVs). We have previously reported a cryo-electron microscopy reconstruction of the ICAM-1:HRV complex (PNAS, 1992) which shows the general features of the binding. Well-diffracting crystals of ICAM-1 expressed in baculovirus are now being used for crystallographic studies. Nevertheless the crystals have somewhat variable cell constants which change by as much as 10 \AA and make MIR phasing problematic. The variability in cell constants is likely attributed to the significant amount of glycosylation. We (Chris Marlor, Jeff Greve; Bayer Inc., W. Haven, CT 06516) have introduced one selenomethionine into ICAM-1 to allow MAD phasing. In addition we are using MAD data collection at the absorption edges of heavy atom derivatives to obtain phase information. We will report the progress of the structure determination of ICAM-1 and its relevance to understanding virus-receptor binding interactions.

The charge surface potentials of several human rhinoviruses have been calculated using X-ray coordinates of HRVs. We have employed site-directed mutagenesis of certain charged residues within the canyon and which overlap with the ICAM-1 footprint determined from the EM reconstruction. The results are consistent with the observed HRV:ICAM-1 interactions.

PS04.09.12 STRUCTURAL STUDIES OF THE ROUS SARCOMA VIRUS (RSV) CAPSID PROTEIN. Ladislav C. Kovari¹, Cory Momany¹, Faith Miyagi¹, Rui Zhao¹, Stephen Campbell², Bao Vong², Volker M. Vogt², Michael G. Rossmann¹, ¹Department of Biological Sciences, Purdue University, West Lafayette, IN 47907, USA, ²Section of Biochemistry, Molecular and Cell Biology, Cornell University, Ithaca, NY 14853, USA

The RSV and HIV virus capsid (CA) proteins exhibit structural and functional similarities. Secondary structural predictions suggest that the two capsid proteins share the same fold. Knowledge of the CA protein structure should prove useful in designing anti-retroviral agents that inhibit viral uncoating, assembly, maturation or release.

Crystals of RSV CA diffract X-rays to 3.5 \AA resolution. The crystals belong to the monoclinic space group C2 with unit cell parameters $a = 374.4 \text{ \AA}$, $b = 128.1 \text{ \AA}$, $c = 200.2 \text{ \AA}$ and $\beta = 121.8^\circ$. An asymmetric unit of the crystal should contain 20 to 30 molecules based on reasonable V_M values. Diffraction data of native and heavy atom derivatives were collected on frozen crystals at home and at CHESS. Self rotation functions suggest that RSV CA crystallizes as a helical array.