

Virus Particle Structures

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COLOR PLATE LEGENDS

These color plates depict the relative sizes and comparative virion structures of multiple types of viruses. The renderings are based on data from published atomic coordinates as determined by X-ray crystallography. The international online repository for 3D coordinates is the Protein Databank (www.rcsb.org/pdb/), maintained by the Research Collaboratory for Structural Bioinformatics (RCSB). The VIPER web site (mmtsb.scripps.edu/viper), maintains a parallel collection of PDB coordinates for icosahedral viruses and additionally offers a version of each data file permuted into the same relative 3D orientation (Reddy, V., Natarajan, P., Okerberg, B., Li, K., Damodaran, K., Morton, R., Brooks, C. and Johnson, J. (2001). *J. Virol.*, **75**, 11943-11947). VIPER also contains an excellent repository of instructional materials pertaining to icosahedral symmetry and viral structures. All images presented here, except for the filamentous viruses, used the standard VIPER orientation along the icosahedral 2-fold axis.

With the exception of Plate 3 as described below, these images were generated from their atomic coordinates using a novel radial depth-cue colorization technique and the program Rasmol (Sayle, R.A., Milner-White, E.J. (1995). RASMOL: biomolecular graphics for all. *Trends Biochem Sci.*, **20**, 374-376). First, the Temperature Factor column for every atom in a PDB coordinate file was edited to record a measure of the radial distance from the virion center. The files were rendered using the Rasmol spacefill menu, with specular and shadow options according to the Van de Waals radius of each atom. Color was assigned on a sliding scale by individual radial distances. The composite assembly and processing used Adobe Photoshop software with attention to relative scale, visual contrast and a uniform color pallet. All graphics are copyright Dr. Jean-Yves Sgro, Institute for Molecular Virology, University of Wisconsin-Madison (E:mail: <jsgro@wisc.edu>) and are available on the VirusWorld web site (virology.wisc.edu/virusworld).

PLATE 1: PICORNAVIRUSES

Bovine enterovirus 1: Picornaviridae; Enterovirus; Bovine enterovirus; strain VG-5-27.

Smyth, M., Tate, J., Hoey, E., Lyons, C., Martin, S. and Stuart, D. (1995). Implications for viral uncoating from the structure of bovine enterovirus. *Nat. Struct. Biol.*, **2**, 224-231. (PDB-ID: 1BEV)

Foot-and-mouth disease virus: Picornaviridae; Aphthovirus; Foot-and-mouth disease virus; strain disease virus.

Fry, E., Acharya, R. and Stuart, D. (1993). Methods used in the structure determination of foot-and-mouth disease virus. *Acta Crystallogr. A*, **49**, 45-55. (PDB-ID: 1BBT)

Human coxsackievirus B3: Picornaviridae; Enterovirus; Human enterovirus B; strain Nancy.

Muckelbauer, J.K., Kremer, M., Minor, I., Diana, G., Dutko, F.J., Groarke, J., Pevear, D.C., Rossmann, M.G. (1995). The structure of coxsackievirus B3 at 3.5 angstrom resolution. *Structure*, **3**, 653-667. (PDB-ID: 1COV)

Human echovirus 1: Picornaviridae; Enterovirus; Human enterovirus B; strain Farouk.

Filman, D.J., Wien, M.W., Cunningham, J.A., Bergelson, J.M. and Hogle, J.M. (1998). Structure determination of echovirus 1. *Acta Crystallogr. D*, **54**, 1261-1272. (PDB-ID: 1EV1)

- Human echovirus 11:** Picornaviridae; Enterovirus; Human enterovirus B; strain 207.
Stuart, A., Mckee, T., Williams, P., Harley, C., Shen, S., Stuart, D., Brown, T. and Lea, S. (2002). Determination of the structure of a decay accelerating factor-binding clinical isolate of echovirus 11 allows mapping of mutants with altered receptor requirements for infection. *J. Virol.*, **76**, 7694-7704. (PDB-ID: 1H8T)
- Human poliovirus 1:** Picornaviridae; Enterovirus; Poliovirus; strain Mahoney Type I.
Miller, S.T., Hogle, J.M. and Filman, D.J. (2003). Crystal structure of Mahoney strain of poliovirus at 2.2A Resolution. (PDB-ID: 1HXS)
- Human rhinovirus 16:** Picornaviridae; Rhinovirus; Human rhinovirus A; strain (NA).
Hadfield, A.T., Lee, W.M., Zhao, R., Oliveira, M.A., Minor, I., Rueckert, R.R. and Rossmann, M.G. (1997). The refined structure of human rhinovirus 16 at 2.15 A resolution: implications for the viral life cycle. *Structure*, **5**, 427-441. (PDB-ID: 1AYM)
- Mengo virus:** Picornaviridae; Cardiovirus; Encephalomyocarditis virus; strain M.
Krishnaswamy, S. and Rossmann, M.G. (1990). Structural refinement and analysis of Mengo virus. *J. Mol. Biol.*, **211**, 803-844. (PDB-ID: 2MEV)
- Theiler's murine encephalomyelitis virus:** Picornaviridae; Cardiovirus; Theilovirus; strain BeAn.
Luo, M., He, C., Toth, K.S., Zhang, C.X. and Lipton, H.L. (1992). Three-dimensional structure of Theiler murine encephalomyelitis virus (BeAn strain). *Proc. Natl. Acad. Sci. USA*, **89**, 2409-2413. (PDB-ID: 1TMF) A10-61.

PLATE 2: COMPARATIVE STRUCTURES

- Adeno-associated virus 2:** *Parvoviridae*; *Dependovirus*; *Adeno-associated virus 2*; strain (recombinant).
Xie, Q., Bu, W., Bhatia, S., Hare, J., Somasundaram, T., Azzi, A. and Chapman, M.S. (2002). Atomic structure of adeno-associated virus (Aav-2), a vector for human therapy. *Proc. Nat. Acad. Sci. USA*, **99**, 10405-10410. (PDB-ID: 1LP3)
- Bean pod mottle virus:** *Comoviridae*; *Comovirus*; *Bean pod mottle virus*; strain Kentucky G7.
Chen, Z.G., Stauffacher, C., Li, Y., Schmidt, T., Bomu, W., Kamer, G., Shanks, M., Lomonosoff, G. and Johnson, J.E. (1989). Protein-RNA interactions in an icosahedral virus at 3.0 A resolution. *Science*, **245**, 154-159. (PDB-ID: 1BMV)
- Bluetongue virus 1, Core:** *Reoviridae*; *Orbivirus*; *Bluetongue virus* (VP3 core protein); serotype 1, South Africa.
Grimes, J.M., Burroughs, J.N., Gouet, P., Diprose, J.M., Malby, R., Zientara, S., Mertens, P.P. and Stuart, D.I. (1998). The atomic structure of the bluetongue virus core. *Nature*, **395**, 470-478. (PDB-ID: 2BTV)
- Brome mosaic virus:** *Bromoviridae*; *Bromovirus*; *Brome mosaic virus*; strain (NA).
Lucas, R.W., Larson, S.B. and McPherson, A. (2002). The crystallographic structure of brome mosaic virus. *J. Mol. Biol.*, **317**, 95-108. (PDB-ID: 1JS9)
- Carnation mottle virus:** *Tombusviridae*; *Carmovirus*; *Carnation mottle virus*; strain (NA).
Morgunova, E.Yu., Dauter, Z., Fry, E., Stuart, D.I., Stel'mashchuk, V.Ya., Mikhailov, A.M., Wilson, K.S. and Vainshtein, B.K. (1994). The atomic structure of carnation mottle virus capsid protein. *FEBS Lett.*, **338**, 267-271. (PDB-ID: 1OPO)
- Cricket paralysis virus 1:** *Dicistroviridae*; *Cripavirus*; *Cricket paralysis virus 1*; strain (NA).
Tate, J., Liljas, L., Scotti, P., Christian, P., Lin, T. and Johnson, J.E. (1999). The crystal structure of cricket paralysis virus: the first view of a new virus family. *Nat. Struct. Biol.*, **8**, 765-774. (PDB-ID: 1B35)
- Canine parvovirus:** *Parvoviridae*; *Parvovirus*; *Canine parvovirus*; strain D Cornell 320 (recombinant empty capsid).
Wu, H. and Rossmann, M.G. (1993). The canine parvovirus empty capsid structure. *J. Mol. Biol.*, **233**, 231-244. (PDB-ID: 2CAS)
- Cucumber mosaic virus:** *Bromoviridae*; *cucumovirus*; *cucumber mosaic virus*; strain Fny.
Smith, T.J., Chase, E., Schmidt, T. and Perry, K. (2000). The structure of cucumber mosaic virus and comparison to cowpea chlorotic mottle virus. *J. Virol.*, **74**, 7578-7586. (PDB-ID: 1F15)
- Enterobacteria phage fd:** *Inoviridae*; *Inovirus*; *Enterobacteria phage fd*;

- Marvin, D.A. (1990). Model-building studies of *Inovirus*: genetic variations on a geometric theme. *Int. J. Biol. Macromol.*, **12**, 125-138. (PDB-ID: 1IFD)
- Enterobacteria phage MS2:** *Leviviridae; Levivirus; Enterobacteria phage MS2*, strain (NA).
Golmohammadi, R., Valegard, K., Fridborg, K. and Liljas, L. (1993). The refined structure of bacteriophage MS2 at 2.8 Å resolution. *J. Mol. Biol.*, **234**, 620-639. (PDB-ID: 2MS2)
- Enterobacteria phage QBeta:** *Leviviridae; Allolevivirus; Enterobacteria phage Q-beta*; strain (NA).
Golmohammadi, R., Fridborg, K., Bundule, M., Valegard, K. and Liljas, L. (1996). The crystal structure of bacteriophage Q-beta at 3.5 Å resolution. *Structure*, **4**, 543-554. (PDB-ID: 1QBE)
- Enterobacteria phage PhiX174:** *Microviridae; Microvirus; Enterobacteria phage phi-X174*, strain (NA).
McKenna, R., Xia, D., Willingmann, P., Ilag, L.L., Krishnaswamy, S., Rossmann, M.G., Olson, N.H., Baker, T.S. and Incardona, N.L. (1992). Atomic structure of single-stranded DNA bacteriophage phiX174 and its functional implications. *Nature*, **355**, 137-143. (PDB-ID: 2BPA)
- Enterobacteria phage PhiX174+scaffold:** *Microviridae; Microvirus; Enterobacteria phage phi-X174*; with scaffold.
Dokland, T., McKenna, R., Ilag, L.L., Bowman, B.R., Incardona, N.L., Fane, B.A. and Rossmann, M.G. (1997). Structure of a viral procapsid with molecular scaffolding. *Nature*, **389**, 308-313. (PDB-ID: 1AL0)
- Galleria mellonella densovirus:** *Parvoviridae; Densovirus; Galleria mellonella densovirus*; strain (NA).
Simpson, A.A., Chipman, P.R., Baker, T.S., Tijssen, P. and Rossmann, M.G. (1998). The structure of an insect parvovirus (*Galleria mellonella densovirus*) at 3.7 Å resolution. *Structure*, **6**, 1355-1367. (PDB-ID: 1DNV)
- Hepatitis B virus:** *Hepadnaviridae; Orthohepadnavirus; Hepatitis B virus*; strain ayw.
Wynne, S.A., Crowther, R.A. and Leslie, A.G.W. (1999). The crystal structure of the human hepatitis B virus capsid. *Molecular Cell*, **3**, 771-780. (PDB-ID: 1QGT)
- Human papillomavirus 16:** *Papillomaviridae; Papillomavirus; Human papillomavirus 16*, strain (recombinant L1 protein).
Modis, Y., Trus, B.L. and Harrison, S.C. (2002). Atomic model of the papillomavirus capsid. *EMBO J.*, **21**, 4754-4762. (PDB-ID: 1LOT)
- Mammalian orthoreovirus 3 - Core:** *Reoviridae; Orthoreovirus; Mammalian orthoreovirus type 3* (LMD1, LMD2, sigma2 core proteins), strain Dearing.
Reinisch, K.M., Nibert, M.L. and Harrison, S.C. (2000). Structure of the reovirus core at 3.6 Å resolution. *Nature*, **404**, 960-967. (PDB-ID: 1EJ6)
- Nodamura virus:** *Nodaviridae; Alphanodavirus; Nodamura virus*, strain (NA).
Zlotnick, A., Natarajan, P., Munshi, S. and Johnson, J.E. (1997). Resolution of space-group ambiguity and the structure determination of Nodamura virus to 3.3 angstrom resolution from pseudo-R32 (monoclinic) crystals. *Acta Crystallogr.*, **53**, 738-746. (PDB-ID: 1NOV)
- Norwalk virus:** *Caliciviridae; Norovirus; Norwalk virus*; strain (recombinant capsid).
Prasad, B.V.V., Hardy, M.E., Dokland, T., Bella, J., Rossmann, M.G. and Estes, M.K. (1999). X-ray crystallographic structure of Norwalk virus capsid. *Science*, **286**, 287-290. (PDB-ID: 1IHM)
- Nudaurelia capensis omega virus:** *Tetraviridae; Omegatetravirus; Nudaurelia capensis omega virus*; strain (NA).
Munshi, S., Liljas, L., Cavarelli, J., Bomu, W., McKinney, B., Reddy, V. and Johnson, J.E. (1996). The 2.8 Å structure of a T=4 animal virus and its implications for membrane translocation of RNA. *J. Mol. Biol.*, **261**, 1-10. (PDB-ID: NA, coordinates available from VIPER)
- Rice dwarf virus:** *Reoviridae; Phytoreovirus; Rice dwarf virus*; strain Akita.
Nakagawa, A., Miyazaki, N., Taka, J., Naitow, H., Ogawa, A., Fujimoto, Z., Mizuno, H., Higashi, T., Watanabe, Y., Omura, T., Cheng, R.H. and Tsukihara, T. (2003). The Atomic structure of rice dwarf virus. *Structure*, **11**, 1227-1238. (PDB-ID: 1UF2)
- Simian virus 40:** *Polyomaviridae; polyomavirus; simian virus 40*; strain (NA).
Stehle, T., Gamblin, S.J., Yan, Y. and Harrison, S.C. (1996). The structure of simian virus 40 refined at 3.1 Å resolution. *Structure*, **4**, 165-182. (PDB-ID: 1SVA)
- Southern bean mosaic virus:** *Sobemovirus; Southern bean mosaic virus*; strain (NA).
Silva, A.M. and Rossmann, M.G. (1987). The refinement of southern bean mosaic virus at 2.9 Å resolution. *J. Mol. Biol.*, **197**, 69-87. (PDB-ID: 4SBV)

- Swine vesicular disease virus:** *Picornaviridae; Enterovirus; Human enterovirus B*; strain UKG/27/72.
Fry, E.E., Knowles, N.J., Newman, J.W.I., Wilsden, G., Rao, Z., King, A.M.Q. and Stuart, D.I. (2003). Crystal structure of swine vesicular disease virus and implications for host adaptation. *J. Virol.*, **77**, 5475-5486. (PDB-ID: 1OOP)
- Tobacco mosaic virus;** *Tobamovirus; Tobacco mosaic virus*; strain vulgare;
Namba, K., Pattanayek, R. and Stubbs, G. (1989). Visualization of protein-nucleic acid interactions in a virus. Refined structure of intact tobacco mosaic virus at 2.9 Å resolution by X-ray fiber diffraction. *J. Mol. Biol.*, **208**, 307-325. (PDB-ID: 2TMV)
- Tobacco necrosis satellite virus;** *Satellite viruses; subgroup 2*; strain (NA).
Jones, T.A. and Liljas, L. (1984). Structure of satellite tobacco necrosis virus after crystallographic refinement at 2.5 Å resolution. *J. Mol. Biol.*, **177**, 735-767. (PDB-ID: 2STV)
- Tobacco necrosis virus;** *Tombusviridae; Necrovirus; Tobacco necrosis virus*; strain A.
Oda, Y., Saeki, K., Takahashi, Y., Maeda, T., Naitow, H., Tsukihara, T. and Fukuyama, K. (2000). Crystal structure of tobacco necrosis virus at 2.25 Å resolution. *J. Mol. Biol.*, **300**, 153-169. (PDB-ID: 1C8N)
- Tomato bushy stunt virus;** *Tombusviridae; Tombusvirus, Tomato bushy stunt virus*; strain BS-3.
Olson, A.J., Bricogne, G. and Harrison, S.C. (1983). Structure of tomato bushy stunt virus IV. The virus particle at 2.9 Å resolution. *J. Mol. Biol.*, **171**, 61-93. (PDB-ID: 2TBV)
- Turnip yellow mosaic virus:** *Tymoviridae; Tymovirus; Turnip yellow mosaic virus*; strain (NA).
Canady, M.A., Larson, S.B., Day, J., McPherson, A. (1996). Crystal structure of turnip yellow mosaic virus. *Nat. Struct. Biol.*, **3**, 771-781. (PDB-ID: 1AUY)

PLATE 3: LARGEST AND SMALLEST VIRAL STRUCTURES. NUCLEIC ACID REVEALED WITHIN PARIACOTO VIRUS.

Both images are rendered to the same relative size scale.

Top: **Paramecium bursaria Chlorella virus 1:** *Phycodnaviridae; Chlorovirus, Paramecium bursaria Chlorella virus 1*; strain (NA), quasi-atomic model.

Nandhagopal, N., Simpson, A., Gurnon, J.R., Yan, X., Baker, T.S., Graves, M.V., van Etten, J.L. and Rossmann, M.G. (2002). The structure and evolution of the major capsid protein of a large, lipid containing, DNA virus. *Proc. Nat. Acad. Sci. USA*, **99**, 14758-14763. (PDB-ID: 1M4X)

Tobacco necrosis satellite virus; *Satellite viruses; subgroup 2*; strain (NA).

Jones, T.A. and Liljas, L. (1984). Structure of satellite tobacco necrosis virus after crystallographic refinement at 2.5 Å resolution. *J. Mol. Biol.*, **177**, 735-767. (PDB-ID: 2STV)

Inset: axial and side views of one trimeric protein unit from Chlorella. Images were created with MOLSCRIPT software (P.J. Kraulis. (1991). MOLSCRIPT: a program to produce both detailed and schematic plots of protein structures. *J. Appl. Cryst.*, **24**, 946-950) then rendered with Raster3D (Merritt, E.A. and Bacon, D.J. (1997). Raster3D: photorealistic molecular graphics. *Meth. Enzymol.*, **277**, 505-524)

Bottom: Left: radial depth-cue molecular surface of a particle of *Pariacoto virus*, split to reveal the dodecahedral arrangement of a portion of the RNA. Right: same image rotated 90°. Both images were rendered using GRASP software. (Nicholls A, Sharp K.A. and Honig B. (1991). Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. *Proteins*, **11**, 281-296)

Pariacoto virus: *Nodaviridae; Alphanodavirus; Pariacoto virus*; strain (NA).

Tang, L., Johnson, K.N., Ball, L.A., Lin, T., Yeager, M. and Johnson, J.E. 2001. The structure of Pariacoto virus reveals a dodecahedral cage of duplex RNA. *Nat. Struct. Biol.*, **8**, 77-83. (PDB-ID: 1F8V)