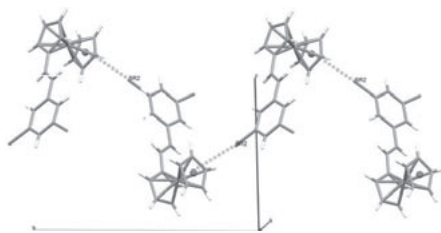


These contacts link molecules into helical coils which are further aggregated to form a network structure. A database search reveals 10 ferrocenyl derivatives displaying similar contacts but only two of these depend solely on the C-Br... $\pi$  interactions for structural stability.



Keywords: ferrocene compounds, crystal engineering, interactions

## MS.28.5

*Acta Cryst.* (2008). A64, C57

### Unexpected patterns in co-crystals of small molecules

Roland Boese, Michael T Kirchner

Universitaet Duisburg-Essen, Institut f. Anorg. Chemie, Universitaetsstr. 5, Essen, NRW, 45117, Germany, E-mail: roland.boese@uni-due.de

Acetylene is a surprisingly good candidate for co-crystallization. It is a reasonable good double proton donor and a good pi-acceptor. The small and rigid molecule is therefore expected to form easy-to-understand primary motifs in the solid state. With mono-functional small proton acceptors such as ethers, carbonyls or alcohols applied as co-crystal partners we thought to find dumbbell-like molecules and with bi-functional partners, linear chains are likely. The same is anticipated with N-containing partners like amines, amides and hetero-aromatic systems. When no acceptor atoms but pi-acceptors are available, we assume that acetylene will prefer C-H... $\pi$  interactions and the formation of chains. But only a few systems obey the rules. Some of the anticipated dumbbell-like molecules are found as zigzag chains, sometimes the acetylene is mono-dentate with dangling hydrogen atoms, and often the geometry does not hold the expectations that lone pair positions are directed towards the hydrogen atoms. In most of the cases, the electrostatic character of these weak hydrogen bonds seems to dominate the geometries and the directionality is less important. Instead, the secondary interaction not only determine the packing but also the question, whether molecular complexes are found or not. Comparison of acetylene complexes with benzene and substituted benzene, e.g. mesitylene, xylene, perfluorobenzene etc. reveals interesting and varying features.

Keywords: cocrystals, hydrogen bonds in organic crystals, crystal engineering

## MS.29.1

*Acta Cryst.* (2008). A64, C57

### X-ray crystallography and HIV vaccine design

Peter D Kwong

National Institutes of Health, NIAID/Vaccine Research Center, 40 Convent Drive - Bldg 40, Room 4508, Bethesda, MD, 20892, USA, E-mail: pdkwong@nih.gov

The human immunodeficiency virus (HIV) has evolved to evade host immune responses. Even after years of infection and elicitation of high levels of HIV-specific antibodies, most HIV infected individuals have ineffective antibodies, which do not neutralize circulating strains of primary HIV. Because HIV is an enveloped virus, the

only viral proteins available to neutralizing antibody reside on the viral spike, which is composed of three copies of the exterior gp120 envelope glycoprotein and three copies of its gp41 transmembrane partner. While the viral spike has resisted atomic-level structure analysis, crystallographic structures of gp120 reveal dense carpets of glycan, evidence for epitope-masking conformational change, and hypervariable surface loops, all of which confirm the challenge of eliciting neutralizing antibody. Despite these difficulties, a few broadly neutralizing antibodies have been identified. We have characterized the structures for two of these antibodies, 2F5 and b12, in complex with their target epitopes. It has been suggested that immunization with precise mimics of these target epitopes might focus the immune response to appropriate sites of vulnerability. X-ray crystallography can assist at each step in the design process, by providing atomic-level mechanisms of evasion, atomic-level descriptions of sites of vulnerability, and structure-based techniques of immunogen design. Progress with each these steps will be presented, with a focus on structure-based immunogen design involving epitope transplantation into both heterologous and homologous scaffolds.

Keywords: immune system, virus host interaction, antibody

## MS.29.2

*Acta Cryst.* (2008). A64, C57

### What we can learn from the structure of viral RNA-dependent RNA polymerases

Nuria Verdaguer

IBMB-CSIC, Structural Biology, Parc Cientific de Barcelona, Baldiri Reixac 10-12, Barcelona, Barcelona, E-08028, Spain, E-mail: nvmcri@ibmb.csic.es

RNA dependent RNA polymerases (RdRPs) are the catalytic components of the RNA replication and the central players in the life cycle of RNA viruses. RdRPs are also a major target for the development of antiviral compounds. RNA viruses are exceptionally diverse in replication strategies, genetic organization, morphology and many other characteristics. Such differences raise significant questions about the diversity of virus origins and the possible extend of functional and evolutionary relationships among existing viruses. These issues are important not only for increasing our basic biological understanding but also for practical applications, since underlying similarities linking virus classes could provide a basis for antiviral approaches that have a broader spectrum. Our recent structural study of a Birnavirus RdRP reveals structural and functional links between positive-strand and double-stranded RNA viruses. We will summarize here the structural and biochemical studies of two different classes of viral RdRPs:

- i) The polymerase 3D of foot-and-mouth disease virus, a member of the Picornaviridae family that possesses a linear plus strand RNA genome.
- ii) The polymerase VP1 of infectious bursal disease virus, a member of the Birnaviridae family with double stranded RNA bipartite genome.

References

- Casanas et al., *Structure*. 2008;16:29-37.  
 Garriga et al., *Proc Natl Acad Sci. USA*. 2007;104:20540-5.  
 Ferrer-Orta et al., *Proc Natl Acad Sci U S A*. 2007; 104:9463-8.  
 Ferrer-Orta et al., *EMBO J*. 2006; 25: 880-8.  
 Ferrer-Orta et al., *Curr. Opin. Struct. Biol*. 2006; 16: 27-34.

Keywords: RNA-dependent RNA polymerase, RNA viruses, viral protein