

## **Report from sessions at ID23**

### **1. Crystal structure of Astrovirus coat protein in complex with HBGAs**

Several datasets of single crystals of Astrovirus coat protein co-crystallized with HBGAs were collected at ID23. The resolution varied between 1.7 Å and 2.1 Å. Molecular replacement was done using the model available from a recent publication (pdb 3QSQ). The spacegroup that was initially calculated from EDNA and xds (C222), but this did not give a usable MR result. Changing the spacegroup to P121 showed a tetramer in the asymmetric unit that fitted well the electron density. No additional electron density was found for any of the investigated carbohydrates.

### **2. Crystal structure of RHDV variant N11 in complex with HBGAs**

Datasets for the P domain of the rabbit hemorrhagic disease virus (RHDV) variant N11 in complex with Lewis Y tetrasaccharide, H2 trisaccharide, and compound 78 were collected at ID23. The single crystals diffracted up to 0.96 Å. Molecular replacement was performed using the autoprocessed EDNA files with an unpublished model of the unliganded N11 P domain. Poor electron density for the fucose moiety of H2tri was visible. The other two ligands didn't show clear patches of electron density.

### **3. Crystal structures of nano-85 in complex with GII.4 P (NSW) domain and GII.4 (Saga) P domain**

Complexes of nano-85 bound to 2 different P domains were crystallized and crystals were obtained after 2 weeks. Crystals of a complex Nano-85 NSW P domain diffracted to 1.9 Å, whereas Nano-85 Saga P domain diffracted to resolution shell of 2 Å. Data processing was performed by EDNA in space group P212121. Molecular replacement was done using apo-structure of a complex nanobody 85 - Vietnam 026 P domain. In all three structures Nano85 bound in identical manner, confirming cross reactivity of Nano-85 with various norovirus strains on a structural level.

### **4. Crystal structure of norovirus NSW Polymerase with ligands**

Norovirus polymerase from NSW strain was soaked with three different drug compounds as well as with RNA primer for three, two and one day. Only crystals soaked for one day diffracted (resolution about 1.6 Å). Data processing was performed using EDNA. Molecular replacement was performed using apo-structure of NSW polymerase previously solved in the laboratory. Refinement is now in process.

### **5. Crystal structure of Fab with GII.4 P-domain**

Fab#7 fragments from commercially available monoclonal antibody were used to form a complex with GII.4 P domain. Crystals of the complex were screened and out of 8 crystals only one diffracted up to 3 Å. Data processing was performed with xds. Structure was solved with molecular replacement using apo-structure of GII.4 P domain and PDB entry 25C8 as models. Preliminary structure of Fab#7 – GII.4 P domain indicated that Fab bound to the region on the P domain that is involved in HBGA binding.

### **6. Crystallization of norovirus shell domain**

GI.10 and GII.4 shell domains were crystallized in 10 different mother liquors and screened for diffraction. Only crystals obtained in C8 (GI.10) and C9 (GII.4) diffracted to

about 5 Å, whereas there was no diffraction observed for any other crystals. Further optimization is required to improve the resolution.