ESRF	Experiment title: Crystallographic data collection on Newcastle disease virus hemagglutinin-neuraminidase and xanthine oxidase.	Experiment number: LS-1683
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Shifts: 3	Local contact(s): Dr Ed Mitchell	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Professor Garry Taylor
Ms Arwen Pearson

Centre for Biomolecular Sciences
University of St Andrews
St Andrews
Fife
KY16 9ST, UK

Report:

Newcastle disease virus (NDV) hemagglutinin-neuraminidase (HN):

The aim of this data collection visit was to obtain as high a resolution data as possible from complexes of NDV HN with various substrates and inhibitors. The NDV HN crystals have always suffered from severe non-isomorphism and in many cases non-isotropic diffraction. Therefore, many crystals were exposed, but only a few gave data of sufficient quality. We were able, however, to collect the highest resolution data ever from HN, 1.85Å, compared with 2.0Å previously. The datasets collected were:

1. **NDV HN from old virus+ 30mM sialyl-lactose (2 week soak). 2.2Å data from 90 frames of data $\Delta\phi$=1°, 90% complete, Rmerge=8.0%.**
2. **NDV HN from new virus+ 15mM sialyl-lactose (1 week soak). 2.4Å data previously collected from this crystal in-house. Data to 1.85Å collected at ESRF, 210° of data, 4 seconds per 1° frame, 95% complete, Rmerge=7.2%.**
3. **NDV HN + 15mM inhibitor. 2.2Å data from 150° of data, 2 seconds per 1° frame, 80% complete, Rmerge=10.2%.**
4. **NDV HN + 15mM inhibitor (Neu5Ac2en). 2.2Å data from 154° of data, 6 seconds per 1° frame, 90% complete, Rmerge=8.3%.**

All datasets reveal electron density for substrate or inhibitor. The sialyl-lactose reveals little density for the lactose, suggesting that there is no recogntion of the sugars preceding the sialic acid. The inhibitor datasets have provided extremely useful information on the key interactions in the active site. The complex structures are all refined to typical HN R-factors of around 22%.

Xanthine oxidase (XO):

We had recently obtained crystals of both the bovine and human milk forms of xanthine oxidase. XO is a dimeric enzyme with three domains in each monomer: a domain with two Fe-S centres, an FAD domain and a domain containing a Mo and pterin cofactor. The dimer has a mass of 300kDa.