EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Calicivirus Interactions with Histo-Blood Group Antigens and Virus Capsid Flexibility (**MNV P domains in complex with HBGAs**)	**Experiment number**: MX1699
Beamline: ID 30A-1	**Date of experiment**: from: 06.02.15 to: 07.02.15	**Date of report**: 08.02.15 (update)
Shifts: 3	**Local contact(s)**: **Bowler, M.**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Grant Hansman
German Cancer Research Center (DKFZ)
Norovirus Study Group – F150
Im Neuenheimer Feld 242
DE – 69120 HEIDELBERG

Report:

Several datasets of single crystals of murine norovirus (MNV) 2007 and CR10 P domains were collected. Diffraction was around 2.8-3Å. Processing of these datasets was succesful but no solution was found during Molecular replacement, even though several different spacegroups were tested.

Datasets for the P domains of the murine norovirus (MNV) variants 2007 and CR10 co-crystallized with B trisachharide, A trisaccharide or sialic acid were collected. The single crystals diffracted up to 3 Å. Processing with xds was succesful. Molecular weight analysis, however, indicated that 10 monomers should be present in the asymmetric unit. Molecular replacement was only succesful with 4 monomers. The solution didn't inidcate the presence of additional electron density for a bound ligand.

ESRF	**Experiment title:** Calicivirus Interactions with Histo-Blood Group Antigens and Virus Capsid Flexibility (Fab fragment bound to RHDV P domain)	**Experiment number**: MX1699
Beamline: ID 30A-1	**Date of experiment**: from: 06.02.15 to: 07.02.15	**Date of report**: 08.02.15 (update)
Shifts: 3	**Local contact(s)**: Bowler, M.	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Grant Hansman
German Cancer Research Center (DKFZ)
Norovirus Study Group – F150
Im Neuenheimer Feld 242
DE – 69120 HEIDELBERG

Report:

10 Crystals of a purified complex of RHDV N11 Pdomain bound to an Fab fragment were tested. Data collection was performed for ~4 crystals. Diffraction was less than 4 Å and EDNA couldn't find a strategy for autoprocessing. Crystal conditions have to be optimized to get better datasets.

ESRF	**Experiment title:** Calicivirus Interactions with Histo-Blood Group Antigens and Virus Capsid Flexibility **(Non-prevalent human Noroviruses interaction with HBGAs)**	**Experiment number**: MX1699
Beamline: ID 30A-1	**Date of experiment**: from: 06.02.15 to: 07.02.15	**Date of report**: 08.02.15 (update)
Shifts: 3	**Local contact(s)**: Bowler, M.	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Grant Hansman
German Cancer Research Center (DKFZ)
Norovirus Study Group – F150
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Report:

Human norovirus P domains from genogroups GII.19 and GII.21 were tested, unbound and co-crystallized with HBGAs. More than 20 datasets were collected and crystals diffracted to better than 2 Å.

Previous results indicated that GII.19 couldn't bind HBGAs due to steric hindrance with the neighbouring unit cell. In a novel attempt we incubated GII.19 P domain with HBGAs prior to crystallization screening. Indeed, the P domain–HBGA mix crystallized under novel conditions.

Analysis of the data however showed, that crystal packing was comparable for all conditions and HBGAs could not bind due to steric hindrance. However, co-crystallization with only the monosaccharide fucose was succesful. Fucose bound to the top of the P domain at a dimeric interface. These results suggested that GII.19 is able to bind HBGAs similar to other NoV variants.

Data collected for GII.21 Pdomain-HBGA complexes are currently under investigation.

ESRF	**Experiment title:** Calicivirus Interactions with Histo-Blood Group Antigens and Virus Capsid Flexibility **(Mutational studies of non-HBGA-binding human noroviruses)**	**Experiment number**: MX1699
Beamline: ID 30A-1	**Date of experiment**: from: 06.02.15 to: 07.02.15	**Date of report**: 08.02.15 (update)
Shifts: 3	**Local contact(s)**: Bowler, M.	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Grant Hansman
German Cancer Research Center (DKFZ)
Norovirus Study Group – F150
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Report:

The prototype genogroup II (GII) norovirus strain, termed Hawai virus (HV) was found not to interact with carbohydrate attachment factors. The reason for that is unknown. In an attempt to restore the binding capability of the HV P domain, we mutated two loops that are close to the carbohydrate binding interface. Crystals of these mutated P domain diffracted to ~1.8 Å. Comparison with the wild-type P domain showed that residues that are possibly involved in ligand interaction, reorientated towards the carbohydrate binding interface.
In addition, we tried to co-crystallize the mutated P domain with carbohydrates. No additional electron denisty was found for bound ligands, from the datasets analyzed so far.