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 using the **Electronic Report Submission Application:**

*http://193.49.43.2:8080/smis/servlet/UserUtils?start*

***Reports supporting requests for additional beam time***

Reports can now 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:** Structural Biology of the Regulation of Bacterial Conjugation | **Experiment number**: MX-480 |
|---|---|---|
| **Beamline**: | **Date of experiment**: from: December 12th to: December 13th | **Date of report**: February 2nd |
| **Shifts:** 1 | **Local contact(s)**: Joanne MCCARTHY | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

**Gabriel Moncalian**

**Dept of Molecular Biology, Universidad de Cantabria, Santander, Spain)**

## Report:

Total number of crystals screened for data collection: 10

Number of crystals from which usable data were measured: 4

Type of Experiment (eg. MAD, SAD, MIR, MR, ...): MAD

For SAD OR MAD experiments:

Anomalous Scatterer: Se and Br

No. of Anomalous scatterers/AU: 4 Se and 2 Br

Wavelengths/Energies used: se inf 0.9793, se peak 0.9791, se remote 0.9756, br inf 0.9198, br peak 0.9194, br remote 0.9168

Approximate crystal dimensions in microns: 0.1

Space Group: P21

Unit Cell: 38.25 92.10 91.90 90.0 91.63 90.0

Data-collection parameters:

Resolution of data collected: 2.5 Å

Exposure time in seconds/frame: 1

Detector Type: ADSC Q210 2D
Data-reduction statistics:

How many complete data sets were recorded? 2 data sets of KorA native crystal, 1 data set at each Inflexion, peak and remote Selenium wavelenghts, 1 data set at each Inflexion, peak and remote Bromine wavelengths of a Se/Br KorA derivative crystal.

Summary of data processing statistics:

Data set processed with mosflm and scala

native

| N | 1/d^2 | Dmin(A) | Rmrg | Rfull | Rcum | Ranom | Nanom | Av_I | SIGMA | I/sigma | sd | Mn(I)/sd | Nmeas | Nref | Ncent | FRCBIAS | Nbias |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $$ | | | | | | | | | | | | | | | | | |
| 1 | 0.0174 | 7.59 | 0.042 | 0.000 | 0.042 | 0.000 | 0 | 112035. | 8457.6 | 13.2 | 6944. | 25.8 | 1797 | 574 | 28 | -0.007 | 646 |
| 2 | 0.0347 | 5.37 | 0.044 | 0.000 | 0.043 | 0.000 | 0 | 84640. | 6690.3 | 12.7 | 5517. | 23.7 | 3467 | 1179 | 28 | -0.010 | 1209 |
| 3 | 0.0521 | 4.38 | 0.050 | 0.000 | 0.047 | 0.000 | 0 | 88857. | 7956.3 | 11.2 | 6249. | 22.4 | 4850 | 1602 | 20 | -0.015 | 1721 |
| 4 | 0.0694 | 3.79 | 0.062 | 0.000 | 0.051 | 0.000 | 0 | 70969. | 7878.4 | 9.0 | 5175. | 20.9 | 5849 | 1915 | 17 | -0.022 | 2089 |
| 5 | 0.0868 | 3.39 | 0.069 | 0.000 | 0.055 | 0.000 | 0 | 48902. | 5988.6 | 8.2 | 3829. | 18.4 | 6738 | 2173 | 19 | -0.030 | 2438 |
| 6 | 0.1042 | 3.10 | 0.081 | 0.000 | 0.058 | 0.000 | 0 | 28351. | 4990.0 | 5.7 | 2589. | 14.6 | 7370 | 2356 | 8 | -0.021 | 2534 |
| 7 | 0.1215 | 2.87 | 0.117 | 0.000 | 0.060 | 0.000 | 0 | 10020. | 1687.4 | 5.9 | 1614. | 8.8 | 7786 | 2454 | 4 | -0.051 | 2851 |
| 8 | 0.1389 | 2.68 | 0.157 | 0.000 | 0.063 | 0.000 | 0 | 6514. | 1458.5 | 4.5 | 1583. | 6.0 | 8284 | 2609 | 2 | -0.088 | 3040 |
| 9 | 0.1562 | 2.53 | 0.235 | 0.000 | 0.066 | 0.000 | 0 | 3931. | 1302.8 | 3.0 | 1588. | 3.8 | 8719 | 2723 | 2 | -0.102 | 3260 |
| 10 | 0.1736 | 2.40 | 0.390 | 0.000 | 0.069 | 0.000 | 0 | 2222. | 1194.6 | 1.9 | 1662. | 2.1 | 9296 | 2903 | 4 | -0.108 | 3535 |

se peak

| N | 1/d^2 | Dmin(A) | Rmrg | Rfull | Rcum | Ranom | Nanom | Av_I | SIGMA | I/sigma | sd | Mn(I)/sd | Nmeas | Nref | Ncent | FRCBIAS | Nbias |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $$ | | | | | | | | | | | | | | | | | |
| 1 | 0.0111 | 9.49 | 0.041 | 0.000 | 0.041 | 0.045 | 287 | 81594. | 5279.4 | 15.5 | 4023. | 30.4 | 756 | 238 | 36 | -0.034 | 229 |
| 2 | 0.0222 | 6.71 | 0.048 | 0.000 | 0.044 | 0.040 | 596 | 43124. | 4583.6 | 9.4 | 2202. | 29.2 | 1478 | 485 | 46 | -0.049 | 479 |
| 3 | 0.0333 | 5.48 | 0.051 | 0.000 | 0.046 | 0.040 | 699 | 21173. | 2094.3 | 10.1 | 1242. | 24.6 | 1658 | 594 | 33 | -0.056 | 678 |
| 4 | 0.0444 | 4.74 | 0.051 | 0.000 | 0.047 | 0.047 | 881 | 19842. | 1860.3 | 10.7 | 1268. | 22.7 | 2308 | 778 | 41 | -0.051 | 808 |
| 5 | 0.0556 | 4.24 | 0.054 | 0.000 | 0.048 | 0.054 | 1018 | 16909. | 1737.9 | 9.7 | 1217. | 20.0 | 2679 | 866 | 40 | -0.043 | 1041 |
| 6 | 0.0667 | 3.87 | 0.066 | 0.000 | 0.050 | 0.058 | 1152 | 12006. | 1427.5 | 8.4 | 1108. | 15.7 | 3078 | 1005 | 38 | -0.050 | 1090 |
| 7 | 0.0778 | 3.59 | 0.077 | 0.000 | 0.053 | 0.068 | 1259 | 9125. | 1124.0 | 8.1 | 1120. | 12.2 | 3429 | 1127 | 44 | -0.052 | 1246 |
| 8 | 0.0889 | 3.35 | 0.091 | 0.000 | 0.056 | 0.079 | 1379 | 7791. | 1182.2 | 6.6 | 1181. | 9.6 | 3723 | 1243 | 46 | -0.047 | 1426 |
| 9 | 0.1000 | 3.16 | 0.105 | 0.096 | 0.060 | 0.080 | 1443 | 7775. | 1775.1 | 4.4 | 1284. | 7.2 | 3889 | 1292 | 44 | -0.027 | 1387 |
| 10 | 0.1111 | 3.00 | 0.198 | 0.000 | 0.064 | 0.177 | 1543 | 2417. | 808.3 | 3.0 | 1095. | 3.5 | 4242 | 1406 | 45 | -0.027 | 1582 |
| $$ | | | | | | | | | | | | | | | | | |

br peak

| N | 1/d^2 | Dmin(A) | Rmrg | Rfull | Rcum | Ranom | Nanom | Av_I | SIGMA | I/sigma | sd | Mn(I)/sd | Nmeas | Nref | Ncent | FRCBIAS | Nbias |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $$ | | | | | | | | | | | | | | | | | |
| 1 | 0.0160 | 7.90 | 0.056 | 0.000 | 0.056 | 0.030 | 567 | 42262. | 4090.8 | 10.3 | 1640. | 40.5 | 1546 | 463 | 60 | 0.011 | 501 |
| 2 | 0.0320 | 5.59 | 0.061 | 0.000 | 0.057 | 0.046 | 929 | 11693. | 1232.5 | 9.5 | 567. | 29.3 | 2180 | 788 | 55 | -0.037 | 768 |
| 3 | 0.0480 | 4.56 | 0.078 | 0.000 | 0.062 | 0.068 | 1265 | 7909. | 1049.8 | 7.5 | 526. | 22.3 | 3332 | 1112 | 58 | -0.012 | 1046 |
| 4 | 0.0641 | 3.95 | 0.101 | 0.000 | 0.068 | 0.084 | 1556 | 4802. | 764.9 | 6.3 | 502. | 15.1 | 4076 | 1315 | 55 | 0.002 | 1282 |
| 5 | 0.0801 | 3.53 | 0.135 | 0.000 | 0.074 | 0.121 | 1768 | 3043. | 650.1 | 4.7 | 546. | 9.0 | 4708 | 1553 | 62 | -0.019 | 1491 |
| 6 | 0.0961 | 3.23 | 0.141 | 0.000 | 0.081 | 0.123 | 2027 | 3079. | 763.2 | 4.0 | 621. | 5.8 | 5402 | 1787 | 64 | -0.026 | 1764 |
| 7 | 0.1121 | 2.99 | 0.283 | 0.000 | 0.088 | 0.271 | 2153 | 1076. | 455.6 | 2.4 | 561. | 2.3 | 5860 | 1934 | 63 | -0.039 | 1873 |
| 8 | 0.1281 | 2.79 | 1.662 | 0.000 | 0.097 | 1.220 | 2302 | 159. | 369.3 | 0.4 | 549. | 0.6 | 6458 | 2145 | 66 | -0.011 | 2085 |
| 9 | 0.1441 | 2.63 | 2.962 | 0.000 | 0.107 | 2.055 | 2474 | 87. | 368.1 | 0.2 | 570. | 0.3 | 6950 | 2334 | 66 | -0.142 | 2345 |
| 10 | 0.1601 | 2.50 | 5.812 | 0.000 | 0.118 | 3.654 | 2638 | 46. | 384.9 | 0.1 | 602. | 0.2 | 7105 | 2377 | 61 | -0.400 | 2445 |

Structure solution (For anomalous scattering experiments only):

If you determined (or attempted to determine) your anomalous sub-structure at ID29, which software did you use?
I am using shelx, BnP, CCP4 and CNS.

Were you able to autotrace your structure?:  Not Yet

Comments on your experience at ID29
The user support and the beamline was excellent. Thank you