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|  | Experiment title: Crystallographic Studies of the Angiopoietin and Tie2 complexes | Experiment number: MX-564 |
| Beamline: ID29 | Date of experiment: from: 2006.07.10 to: 2006.07.10 | Date of report: 2007.01.02 <i>Received at ESRF:</i> |
| Shifts: 2 | Local contact(s): John Mcgeehan | |
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Report:

We have conducted the following two experiments using the beam time allocated.

(1) Crystallographic studies of the angiopoietin-tie2 complexes.

The angiopoietin2-tie2 complex crystals diffracted x-ray to 2.9 angstrom resolution. A native data set and two derivative data sets have been collected at the ID29 beamline. The structure is determined by the molecular replacement technique and the manuscript is being prepared.

Summary of the data collection

| | Native | Gold | Lead |
|------------------------------------|-------------------|-----------------|-------------------|
| Space group | P2 ₁ | P2 ₁ | P2 ₁ |
| Cell dimensions | | | |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 98.1 92.5 108.4 | 97.6 91.7 107.8 | 97.2 88.9 106.9 |
| α , β , γ (°) | 90.0, 104.6, 90.0 | 90. 104.8 90. | 90.0, 105.0, 90.0 |
| Resolution (Å) | 2.9 | 2.9 | 3.5 |
| <i>R</i> _{sym} | 9.0 (28.7)* | 7.9 (14.1)* | 11.3 (14.8)* |
| <i>I</i> / σ <i>I</i> | 12.6 (2.6)* | 11.6 (3.4)* | 6.7 (4.0)* |
| Completeness (%) | 90.1 (61.5)* | 80.8 (51.5)* | 83.2 (76.5)* |
| Redundancy | 4.3 | 2.1 | 2.2 |

(2) Crystallographic studies of the hagfish VLR receptors.

This work has been accepted for publication in the Journal of the Biological Chemistry.

Title: Structural Diversity of the Hagfish Variable Lymphocyte Receptors.

Abstracts:

Variable Lymphocyte Receptors (VLRs) are recently-discovered Leucine Rich Repeat (LRR) family proteins that mediate adaptive immune responses in jawless fish. Phylogenetically it is the oldest adaptive immune receptor and the first one with a non-immunoglobulin fold. We present the crystal structures of one VLR-A and two VLR-B clones from the inshore hagfish. The hagfish VLRs have the characteristic horseshoe shaped structure of LRR family proteins. The backbone structures of their LRR modules are highly homologous and the sequence variation is concentrated in the concave surface of the protein. The conservation of key residues suggests that our structures are likely to represent the LRR structures of the entire repertoire of jawless fish VLRs. The analysis of sequence variability, prediction of protein interaction surfaces, amino acid composition analysis and structural comparison with other LRR proteins, suggest that the hypervariable concave surface is the most probable antigen binding site of the VLR.

Summary of the data collection and refinement

| | Eb7VLRA.29 | Eb8VLRB.59 | Eb8VLRB.61 |
|---|--------------------|------------------|---|
| Data collection | | | |
| Space group | P3 ₂ 21 | P1 | P2 ₁ 2 ₁ 2 ₁ |
| Cell dimensions | | | |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 95.2, 95.2, 77.5 | 30.7, 50.0, 69.4 | 42.8, 55.4, 81.1 |
| α , β , γ (°) | 90.0, 90.0, 120.0 | 69.2, 76.9, 86.1 | 90.0, 90.0, 90.0 |
| Resolution (Å) | 2.5 | 1.5 | 2.3 |
| <i>R</i> _{sym} | 9.0 (28.7)* | 4.5 (10.2)* | 4.8 (5.0)* |
| <i>I</i> / σ <i>I</i> | 12.6 (2.6)* | 28.7 (13.9)* | 86.5 (41.7)* |
| Completeness (%) | 91.0 (61.5)* | 91.2 (84.6)* | 93.6 (68.7)* |
| Redundancy | 4.3 | 3.7 | 4.8 |
| Refinement | | | |
| Resolution (Å) | 20-2.5 | 20-1.5 | 20-2.3 |
| No. reflections (work/test) | 12265/663 | 49294/5557 | 7557/877 |
| <i>R</i> _{work} / <i>R</i> _{free} | 22.5/26.2 | 19.6/21.5 | 19.1/25.9 |
| No. atoms (in asymmetric unit) | | | |
| Protein | 2110 | 3201 | 1375 |
| Water | 215 | 336 | 191 |
| <i>B</i> -factors | | | |
| Protein | 40.7 | 9.9 | 12.4 |
| Water | 51.0 | 21.1 | 26.2 |
| R.m.s deviations | | | |
| Bond lengths (Å) | 0.0097 | 0.006 | 0.011 |
| Bond angles (°) | 1.61 | 1.44 | 1.82 |