Here is a cumaltive report from several sessions at ID23-1, ID14-1, and ID29

HBGAs bound crystal structures of Saga P domain

All the HBGAs bound crystals of Saga P domain were crystallized in the space group C 1 2 1. Crystals had two ligands bound to a Saga P domain dimer per assymetric unit. The complex structures were solved by molecular replacement (MR) using the native Saga P domain monomer structure as the initial model. The composition and overall structural topology of Saga P-domain were well conserved among all complex structures.

1. Saga P domain-A-trisaccharide complex

Dataset for a single crystal of A-trisacchaaride bound Saga P domain was processed at 1.28Å resolution with completeness 92.1%. The matthew co-efficient for this crystal was 2.15 that corresponded to 42.76% solvent content. The electron density difference map (F_o-Fc) for bound A-trisacchaaride was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1920 and 0.2090, respectively, and well-defined electron density for all saccharide rings. The electron density map ($2F_o$-Fc) map for the terminal fucose ring was strongest while that for the other two saccharide rings was weaker progressively. Further refinement to reduce R-factors is in progress.

2. Saga P domain-B-trisaccharide complex

Dataset for a single crystal of B-trisacchaaride bound Saga P domain was processed at 1.25Å resolution with completeness 97.2%. The matthew co-efficient for this crystal was 2.15 that corresponded to 42.73% solvent content. The F_o-Fc map for all the saccharide rings of bound B-trisacchaaride was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1334 and 0.1578, respectively. The $2F_o$-Fc map for a flexible loop between residues 391-395 was poorely defined in HBGAs bound and unbound Saga P domain structures. Interestingely, two different orientations of this loop region had been observed in this complex structure.

3. Saga P domain- Lewis^a- trisaccharide

Dataset for a single crystal of Lewis^a-trisaccharide bound Saga P domain was processed at 1.59Å resolution with completeness 98.3%. The matthew co-efficient for this crystal was 2.18 that corresponded to 43.51% solvent content. The F_o-Fc map for only the terminal fucose ring of bound Lewis^a-trisaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1860 and 0.2098, respectively. The $2F_o$-Fc map for the remaining two saccharide rings of Lewis^a-trisaccharide was so weak that saccharides could not be fitted in.

4. Saga P domain- Lewis^b- tetrasaccharide

Dataset for a single crystal of Lewis^b-tetrasaccharide bound Saga P domain was processed at 1.38Å resolution with completeness 99.3%. The matthew co-efficient for this crystal was 2.15 that corresponded to 42.72% solvent content. The F_o-Fc map for all the saccharide rings of bound Lewis^b-tetrasaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1602 and 0.1860, respectively. Further refinement is in progress to gain optimal R-factors. In this complex structure, the loop region between the residues 291-295 interacted directly with Lewis fucose Lewis^b-tetrasaccharide, playing a crucial role in stabliizng binding of Lewis^b-tetrasaccharide in HBGA binding pocket. In addition, this interaction also reduced flexibility of this loop that resulted in a well-defined electron density for this region.

5. Saga P domain- Lewis^{Y}- tetrasaccharide

Dataset for a single crystal of Lewis^{Y}-tetrasaccharide bound Saga P domain was processed at 1.60Å resolution with completeness 91.3%. The matthew co-efficient for this crystal was 2.18 that corresponded to 43.49% solvent content. The F_o-Fc map of bound Lewis^{Y}-trisaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1908 and 0.2030, respectively, and well-defined electron density for all saccharide rings. The $2F_o$-Fc map for the terminal fucose ring was strongest while that for the other three saccharide rings was weaker progressively. In this structure the loop region between the residues 291-295 was re-oriented to accommodate saccharide rings of Lewis^{Y}-tetrasaccharide in the HBGA binding pocket.

6. Saga P domain- H-type 2 trisaccharide

Dataset for a single crystal of H-type 2 trisaccharide bound Saga P domain was processed at 1.47Å resolution with completeness 97.4%. The matthew co-efficient for this crystal was 2.15 that corresponded to 42.69% solvent content. The F_o-Fc map for all the three saccharides of bound H-type 2 trisaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1309 and 0.1649, respectively, and well-defined electron density for all saccharide rings.

HBGAs bound and native crystal structures of UNSW P domain

All the HBGAs bound crystals of UNSW P domain were crystallized in the space group P 41 21 2 with a two-ligands bound dimer per assymetric unit, while the crystal of native UNSW P domain was crystallized in the space group C 1 2 1 as monomer per assymetric unit. The native structure UNSW P domain was determined by MR using the native Saga P domain monomer structure as the initial model. The complex structures were solved by MR using the native UNSW P domain monomer structure as the initial model. The composition and overall structural topology of UNSW P-domain are well conserved among native and complex structures.

1. UNSW P domain

Dataset for a single crystal of UNSW P domain was processed at 1.60Å resolution with completeness 98.1%. The matthew co-efficient for this crystal was 2.14 that corresponded to 42.69% solvent content. Refinement led to the R_{work} and R_{free} values 0.1505 and 0.1762, respectively.

2. UNSW P domain- A-trisaccharide

Dataset for a single crystal of A-trisaccharide bound UNSW P domain was processed at 1.85Å resolution with completeness 98.8%. The matthew co-efficient for this crystal was 2.24 that corresponded to 45.02% solvent content. The F_o-Fc map for all the three saccharides of bound A-trisaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1629 and 0.1899, respectively, and well-defined electron density for all saccharide rings.

3. UNSW P domain- B-trisaccharide

Dataset for a single crystal of B-trisaccharide bound UNSW P domain was processed at 1.92Å resolution with completeness 93.8%. The matthew co-efficient for this crystal was 2.24 that corresponded to 45.02% solvent content. The F_o-Fc map for all the three saccharides of bound B-trisaccharide was observed after molecular replacement.

Refinement led to the R_{work} and R_{free} values 0.1882 and 0.2135, respectively, and well-defined electron density for all saccharide rings.

4. UNSW P domain- Lewis^x trisaccharide

Dataset for a single crystal of Lewis^x-trisaccharide bound UNSW P domain was processed at 1.72Å resolution with completeness 99.3%. The matthew co-efficient for this crystal was 2.20 that corresponded to 44.06% solvent content. The F_o-Fc map of bound Lewis^x-trisaccharide was observed after molecular replacement. Refinement led to the R_{work} and R_{free} values 0.1649 and 0.1825, respectively. The $2F_o$-Fc map for terminal fucose and glucosamine pyronose rings was well defined while that for galactose was weakely defined.