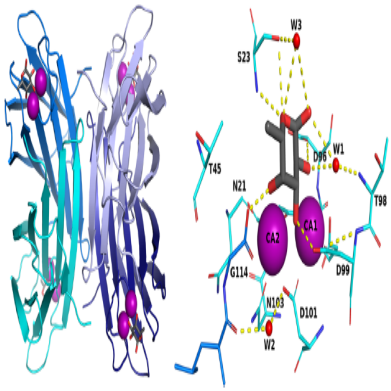
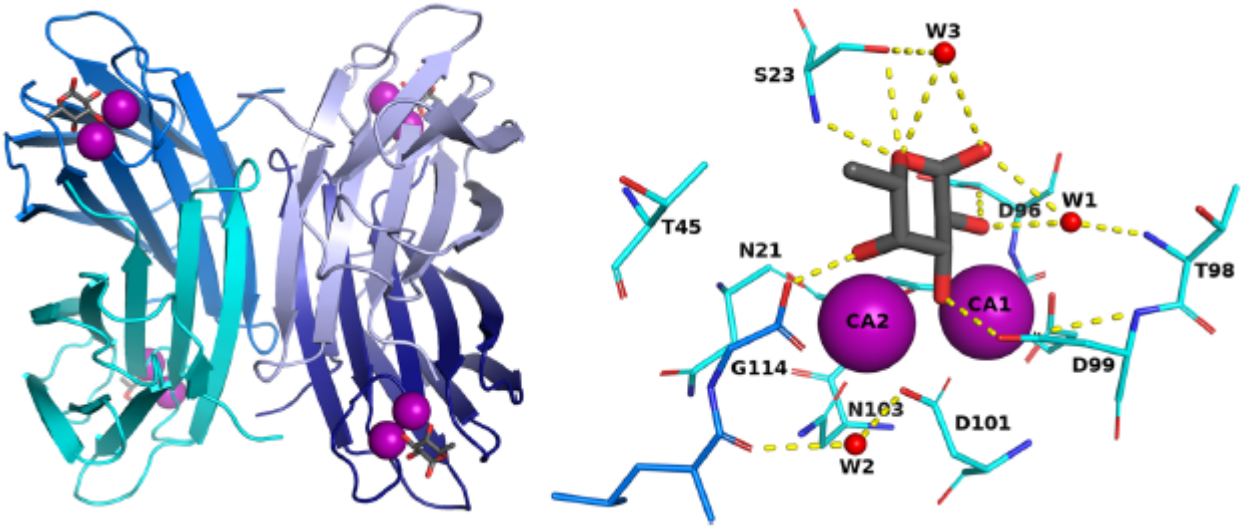


Neutron crystallography reveals mechanisms used by Pseudomonas aeruginosa for host-cell binding

Description

The opportunistic pathogen *Pseudomonas aeruginosa*, a major cause of nosocomial infections, uses carbohydrate-binding proteins (lectins) as part of its binding to host cells. The fucose binding lectin, LecB, displays a unique carbohydrate-binding site that incorporates two closely located calcium ions bridging between the ligand and protein, providing specificity and unusually high affinity. The authors investigate the mechanisms involved in binding based on neutron crystallography studies of a fully deuterated LecB/fucose/calcium complex.



The neutron structure, which includes the positions of all the hydrogen atoms, reveals that the high affinity of binding may be related to the occurrence of a low-barrier hydrogen bond induced by the proximity of the two calcium ions, the presence of coordination rings between the sugar, calcium and LecB, and the dynamic behaviour of bridging water molecules at room temperature. These key structural details may assist in designing anti-adhesive compounds to combat multi-resistance bacterial infections.

Category

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