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## Data Article

## A complex water network contributes to high-affinity binding in an antibody–antigen interface



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## ABSTRACT

This data article presents an analysis of structural water molecules in the high affinity interaction between a potent tumor growth inhibiting antibody (fragment), J22.9–xi, and the tumor marker antigen CD269 (B cell maturation antigen, BCMA). The 1.89 Å X-ray crystal structure shows exquisite details of the binding interface between the two molecules, which comprises relatively few, mostly hydrophobic, direct contacts but many indirect interactions over solvent waters. These are partly or wholly buried in, and therefore part of, the interface. A partial description of the structure is included in an article on the tumor inhibiting effects of the antibody: “Potent anti-tumor response by targeting B cell maturation antigen (BCMA) in a mouse model of multiple myeloma”, *Mol. Oncol.* 9 (7) (2015) pp. 1348–58.

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## Specifications Table

Subject area	<i>Chemistry, Biology, Cancer immunology</i>
More specific subject area	<i>Structural biology</i>
Type of data	<i>Parameter table for structurally observed water molecules; figures depicting positions of these waters in a binding interface</i>
How data was acquired	<i>Analysis of the refined X-ray crystallographic structure.</i>
Data format	<i>Table, figures.</i>

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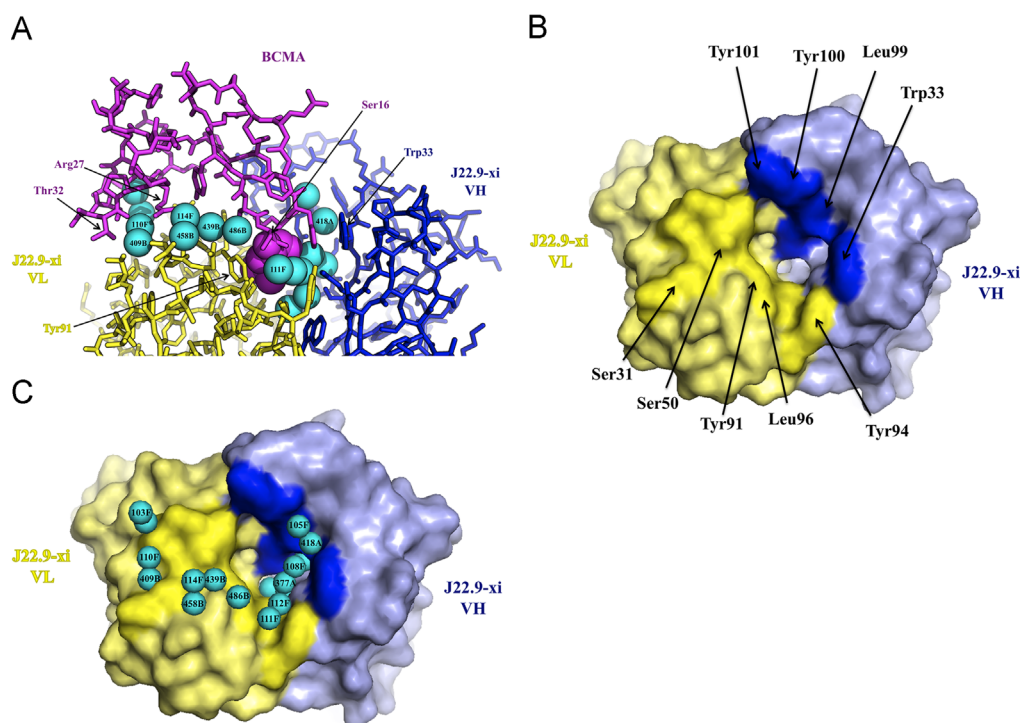
<http://dx.doi.org/10.1016/j.dib.2015.12.023>

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Experimental factors	<i>Fab fragments from anti-CD269 (BCMA) IgGs co-crystallized with antigen and the structure solved to high (1.89 Å) resolution</i>
Experimental features	<i>Interface interactions in the refined structure were assessed and the contribution of water to the binding evaluated.</i>
Data source location	<i>Protein Data Bank</i>
Data accessibility	<a href="http://www.rcsb.org/pdb/home/home.do">http://www.rcsb.org/pdb/home/home.do</a> (PDB code: 4ZFO)

## Value of the data

- The antibody targets the very restrictively expressed tumor marker BCMA for Multiple Myeloma and potently inhibits tumor growth in mice
- The antibody has an exceptionally high affinity to BCMA (picomolar)
- The high resolution crystal structure of the antibody-BCMA complex reveals a network of water molecules in the binding interface
- The structure shows how very high affinity can be achieved with a minimal number of direct protein-protein contacts



**Fig. 1.** Water molecules in the J22.9-xi binding site. **A.** A view of the binding interaction between BCMA (magenta) and the variable domains of the heavy chain (VH, blue) and light chain (VL, yellow). Interface water molecules participating in bridging hydrogen bonding interactions between BCMA and J22.9-xi are depicted as cyan spheres with a radius of 1.4 Å. For clarity only some interface residues (with the corresponding chain color) and some interface waters (with chain numbers directly on the spheres) are labeled. Leu17 in the BCMA D<sub>x</sub>L loop is shown in space-filling representation. **B.** A view looking down on the binding cavity in J22.9-xi with BCMA removed. The Fab fragment is shown in surface representation with the heavy chain colored blue and the light chain colored yellow. Some of the residues making direct contacts to BCMA are indicated with arrows and darker coloring. **C.** View as in (B) with interface waters depicted as cyan spheres and labeled as in (A).

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