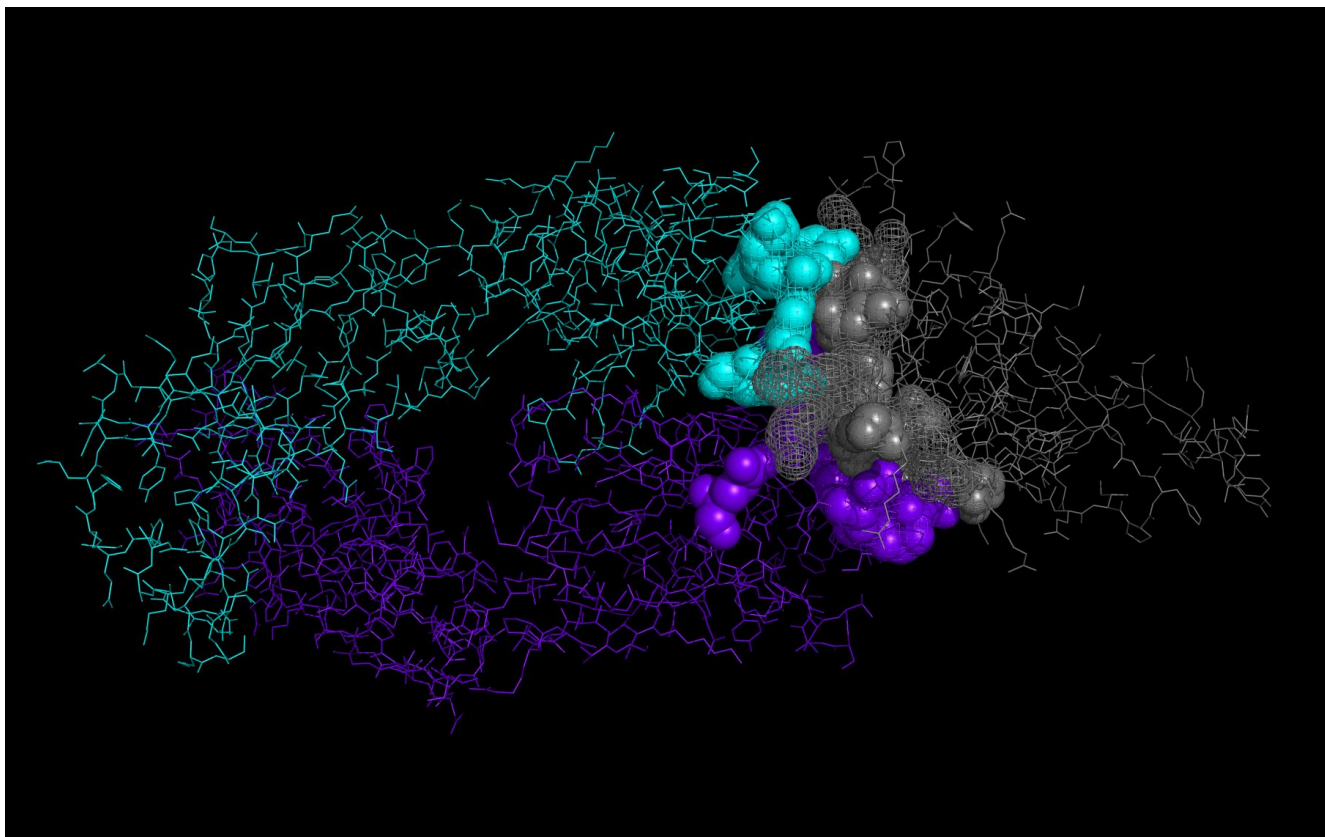


**Weininger, A.; Weininger S.**  
**“Finding antigen features in an antigen-antibody interface”**  
*Weininger Works Technical Notes (2013) Jul 13;1:1-12*



**Basiliximab/IL-2 contacting residues**

Shown here is the crystal structure<sup>1</sup> of basiliximab binding to IL-2 overlaid with spheres representing atoms identified by wwavePDB analysis that form the contact surface between basiliximab and IL-2.

wwavePDB *identifies* the atoms forming the Ab/Ag contact surface and *delivers* detailed, easy to display information on the components and structure of the contact.

wwavePDB-identified contact atoms fill out volumes represented here by mesh surfaces:

- purple surface encloses atoms in residues from the basiliximab H-chain that contact IL-2
- cyan surface encloses atoms in residues from the basiliximab L-chain that contact IL-2
- grey surface encloses atoms in residues from IL-2 that contact basiliximab

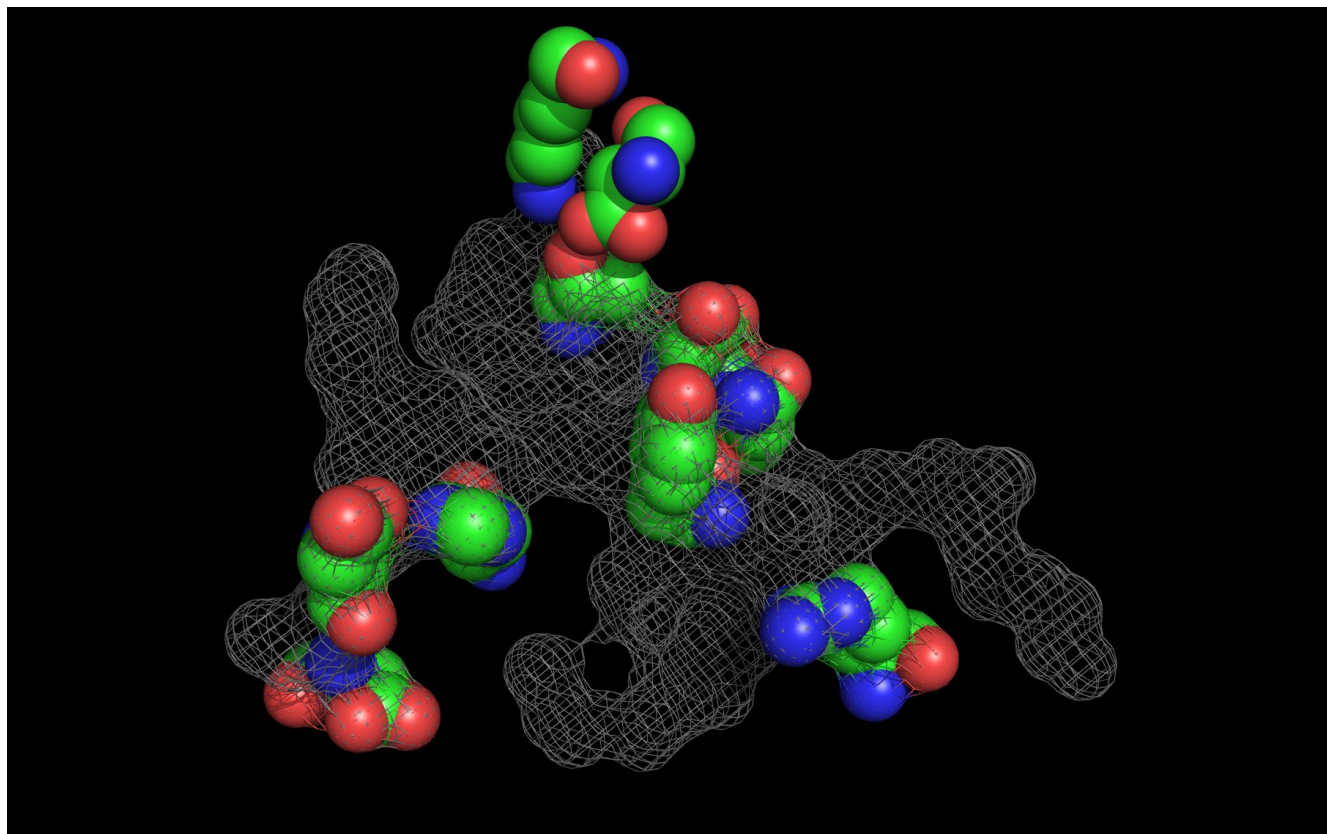
Basiliximab (Simulect; Novartis Pharmaceuticals, East Hanover, NJ) is an approved (1998) therapeutic antibody in the same class as daclizumab (Zenapax; Roche, Basel, Switzerland).

<sup>1</sup> Protein Data Bank ID: 3IU3.

Du; H. Yang; D. Zhang; J. Wang; H. Guo; B. Peng; Y. Guo; J. Ding;

“Structural basis for the blockage of the IL-2 signaling by therapeutic antibody basiliximab”

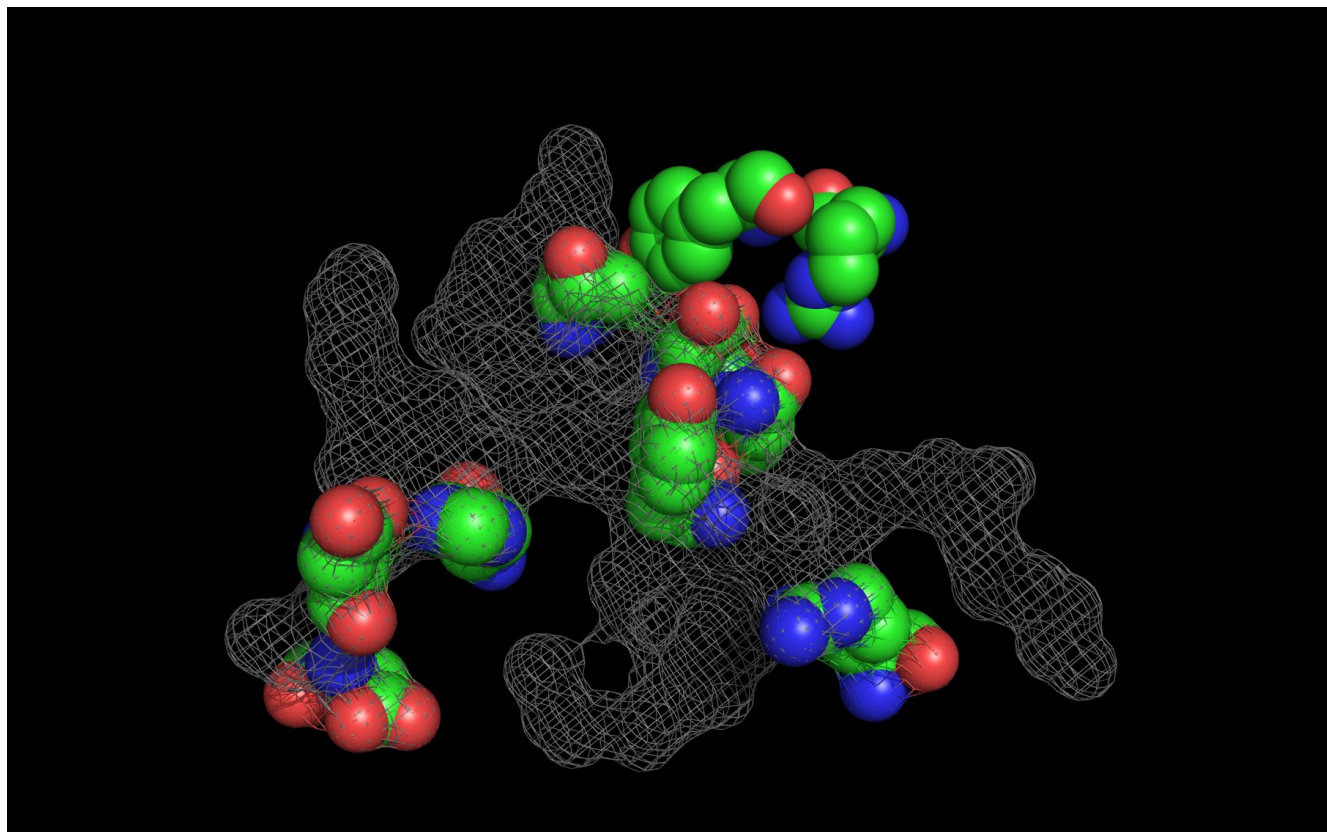
*Immunology* (2010) 184(3): 1361-1368



### **Basiliximab L chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab L chain residues ASP49 and LYS52 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

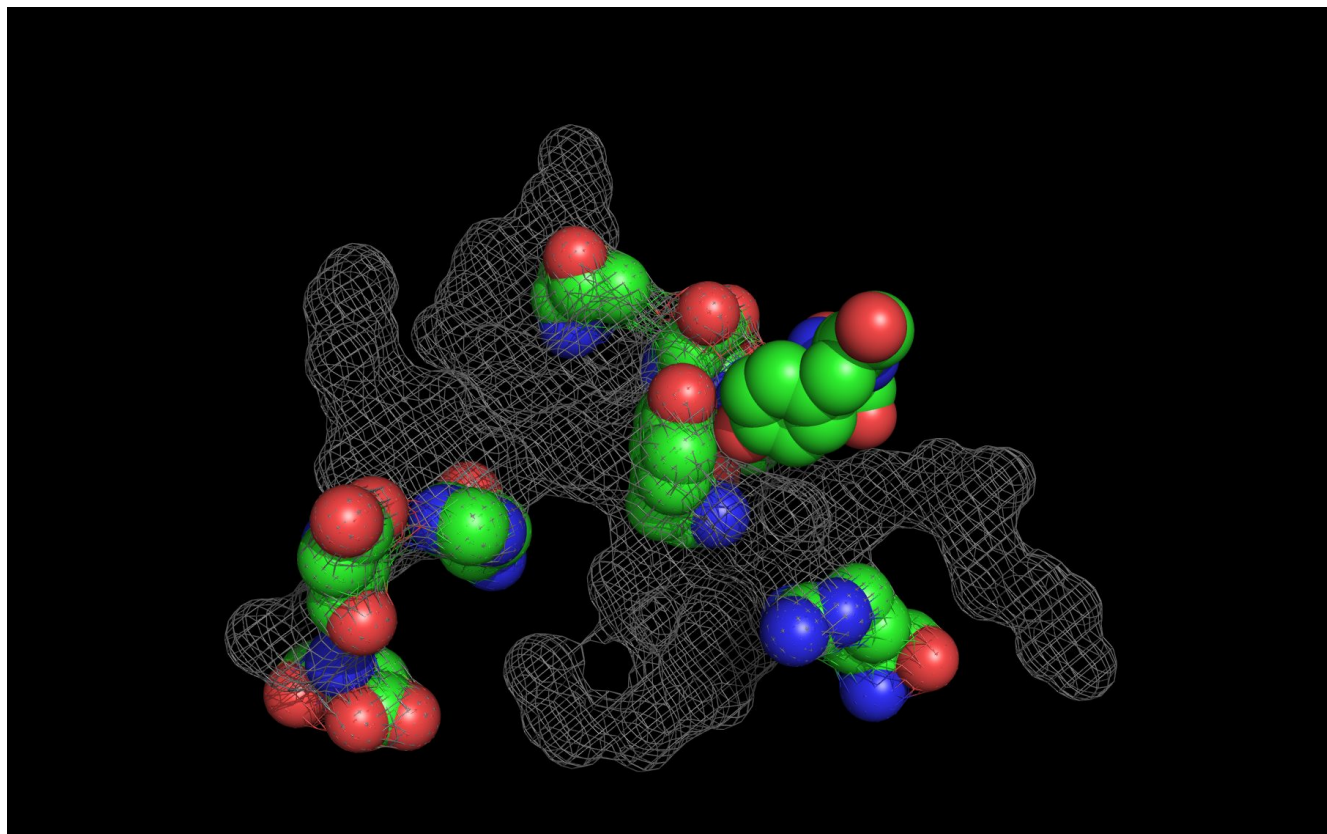
The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **Basiliximab L chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab L chain residues ARG29 and TYR31 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).

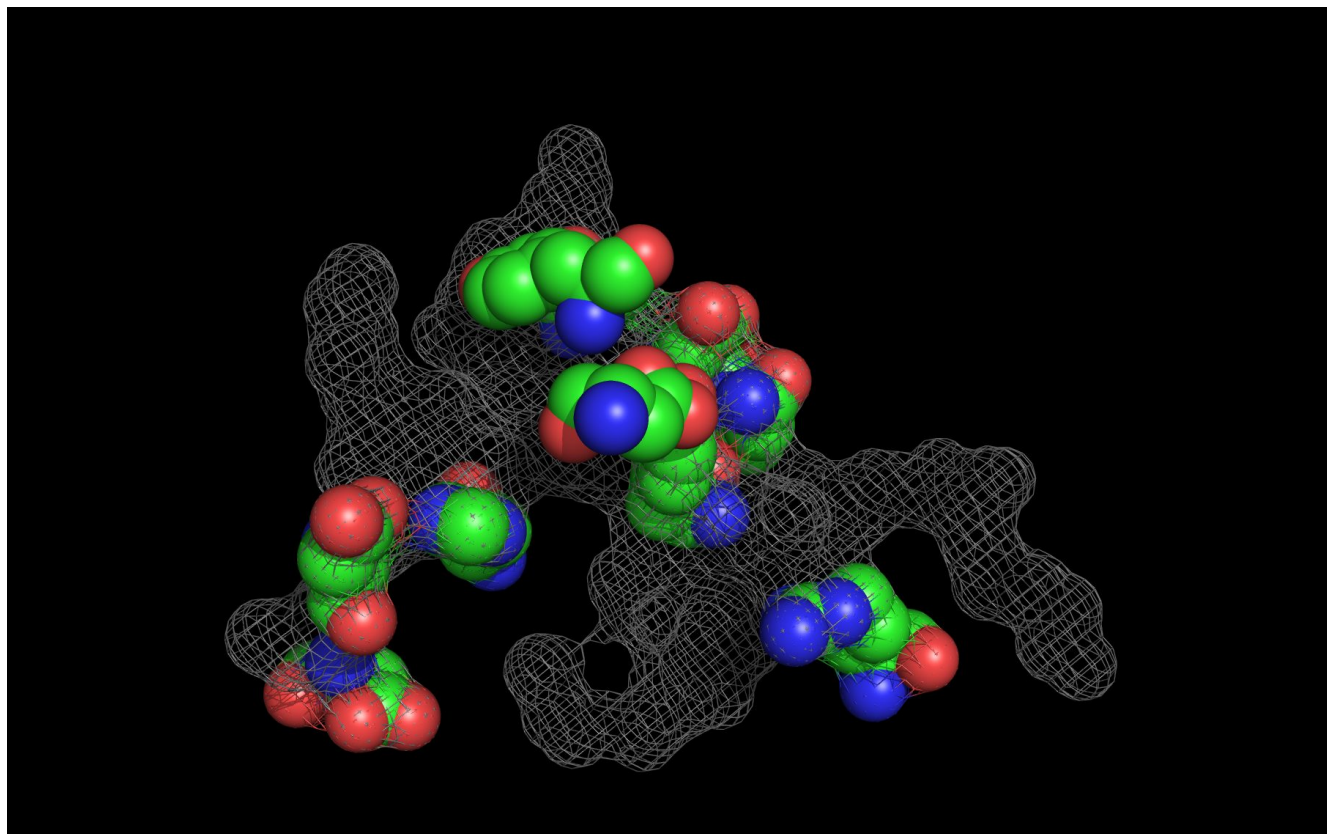


### **Basiliximab L chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab L chain residues SER91 and TYR93 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).

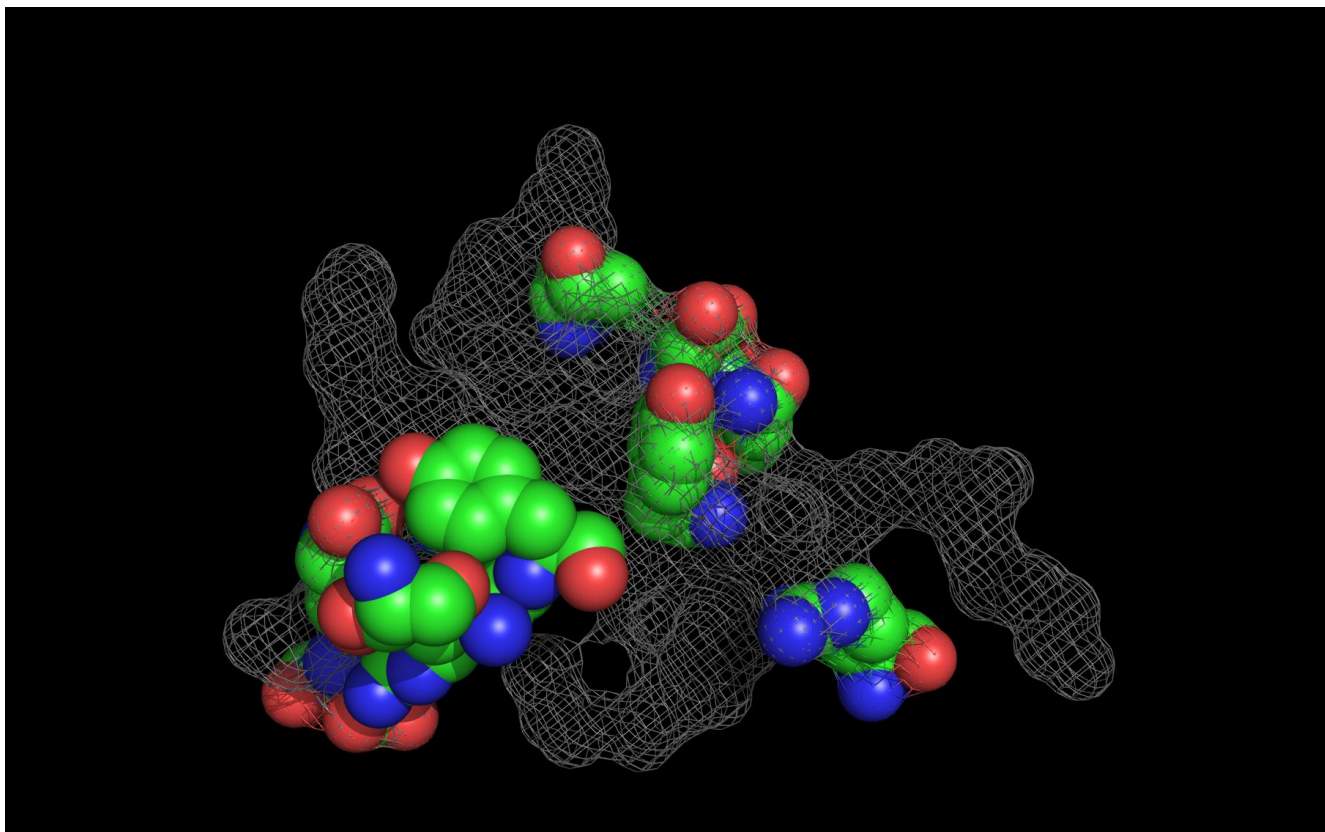




### **Basiliximab H chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab H chain residues ASP97 and TYR100 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

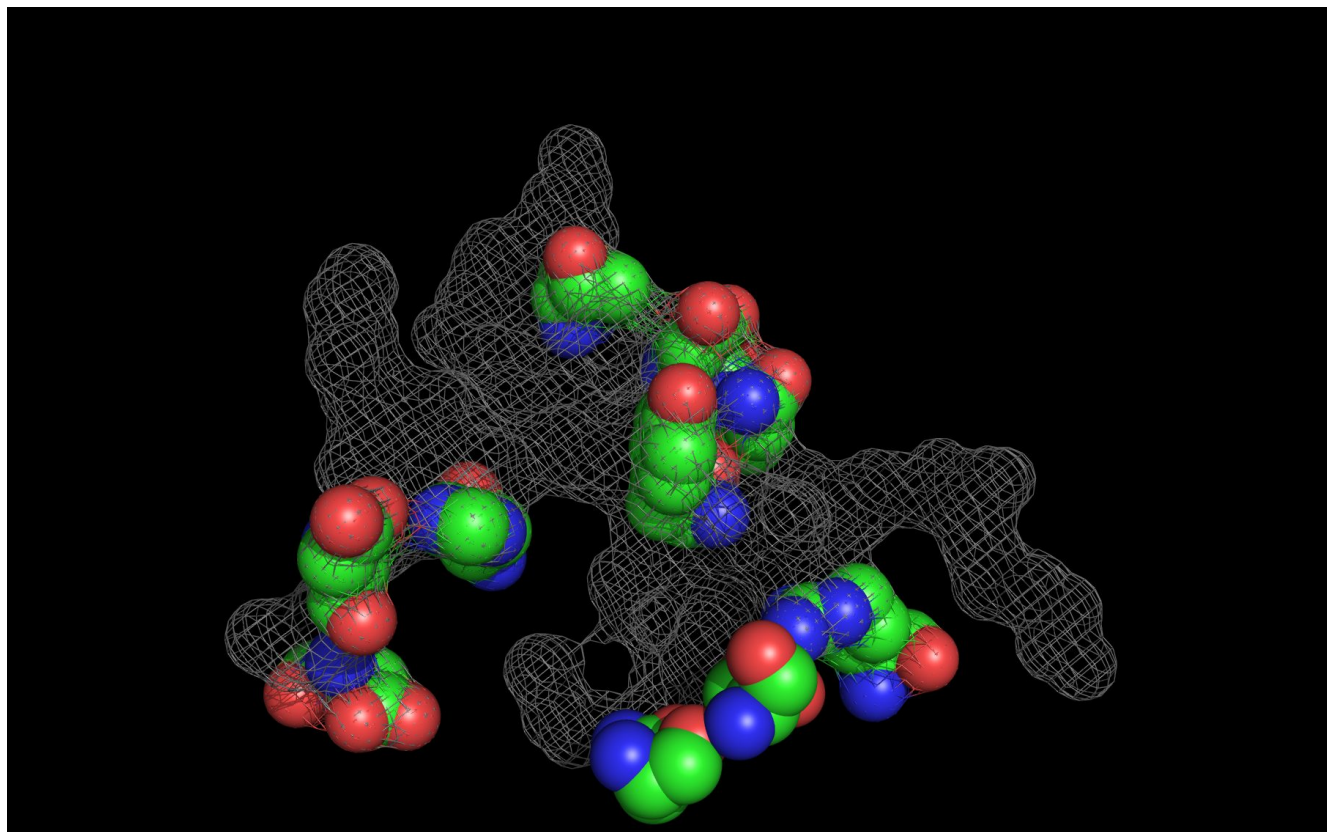
The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **Basiliximab H chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab H chain residues SER26, ARG29, and TYR30 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

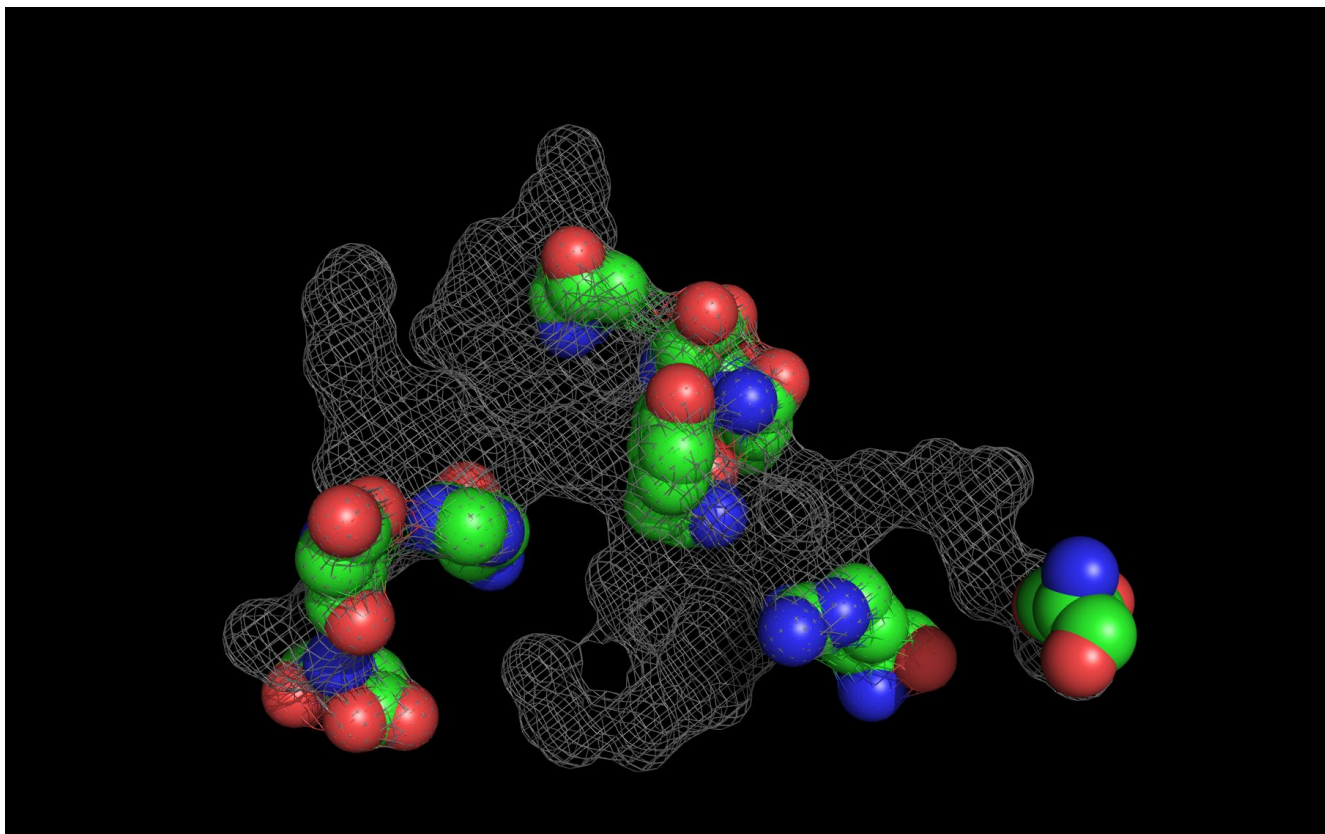
The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **Basiliximab H chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab H chain residues ASN53 and ASP55 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).

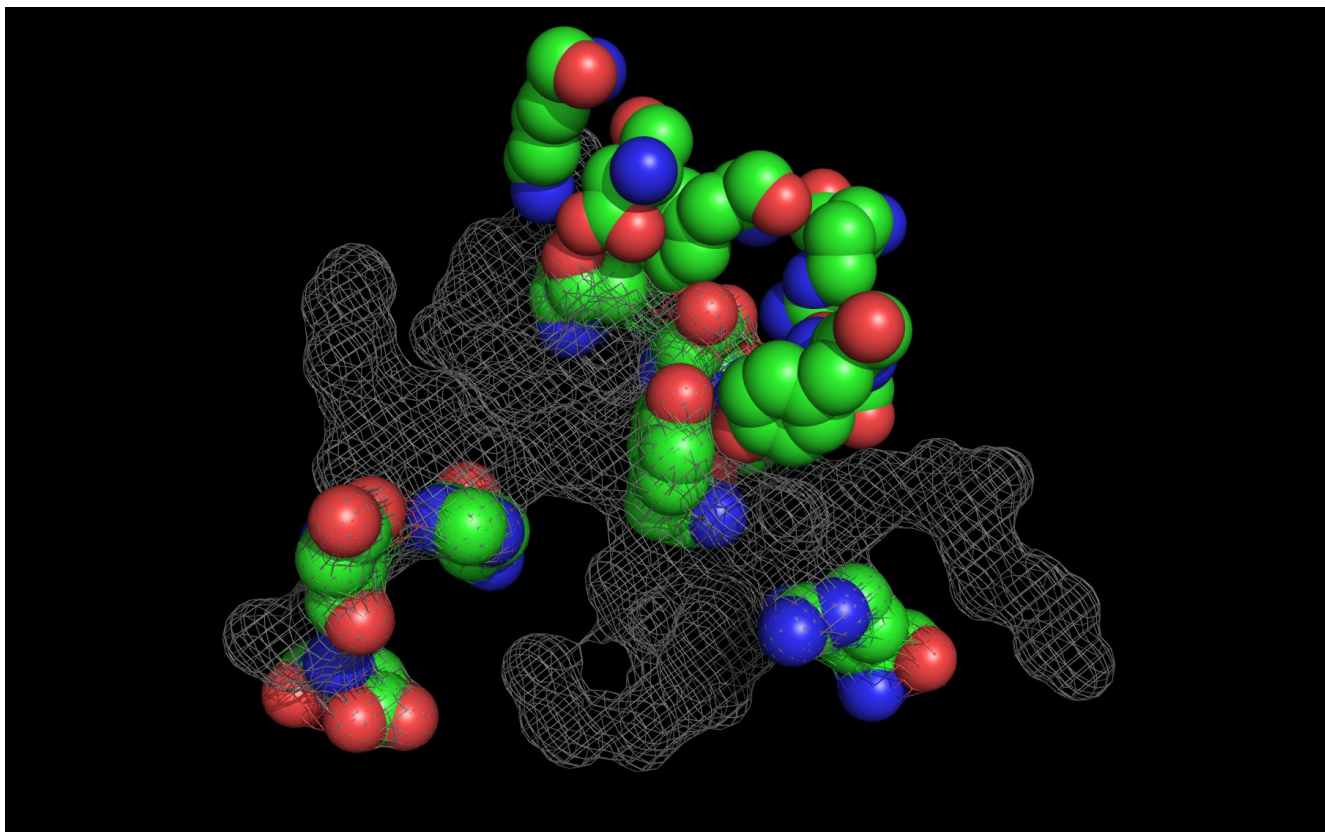


### **Basiliximab H chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab H chain residue GLU63 is shown contacting the IL2 contact volume.

The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).

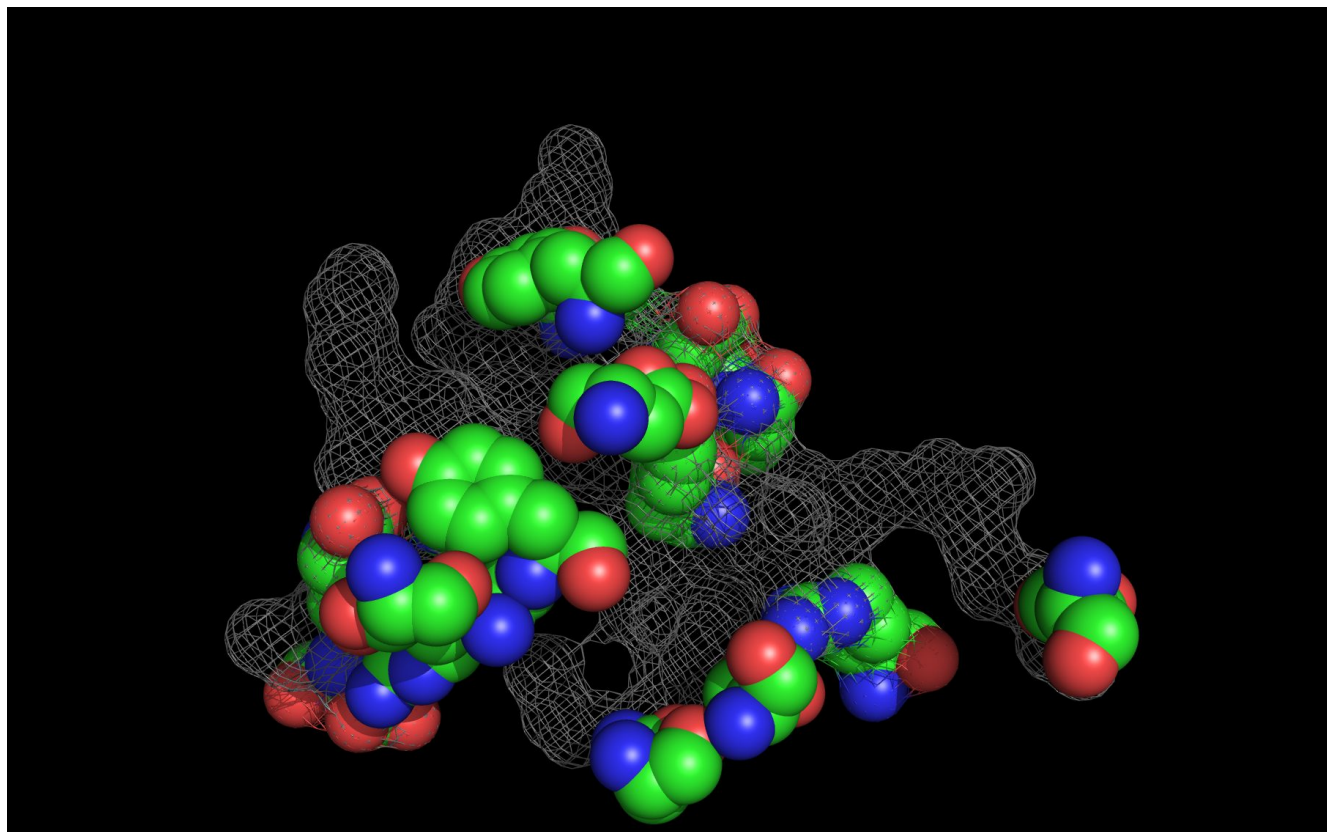




### **Basiliximab L chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab L chain residues ARG29, TYR31, ASP49, LYS52, SER91 and TYR93 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

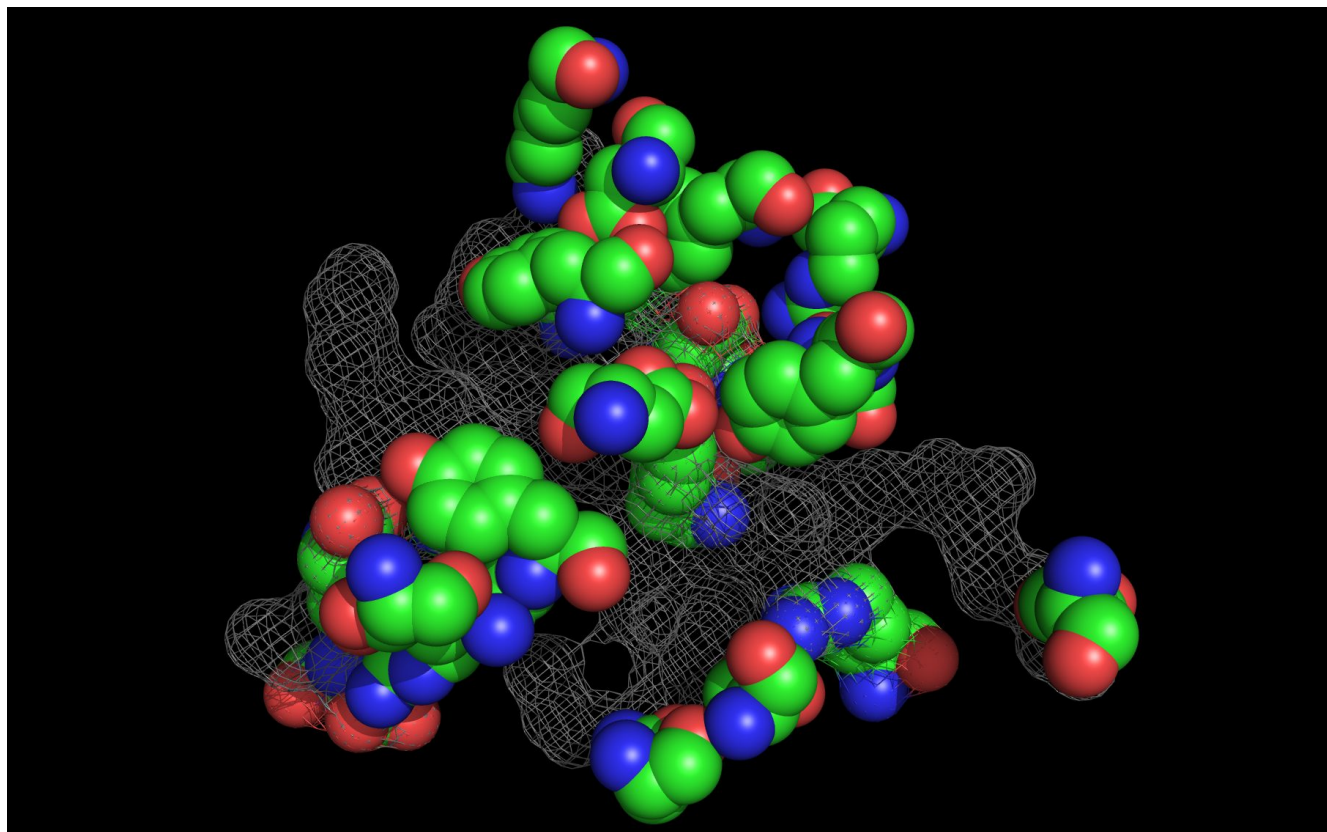
The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **Basiliximab H chain residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab H chain residues SER26, ARG29, TYR30, ASN53, ASP55, GLU63, ASP97, and TYR100 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

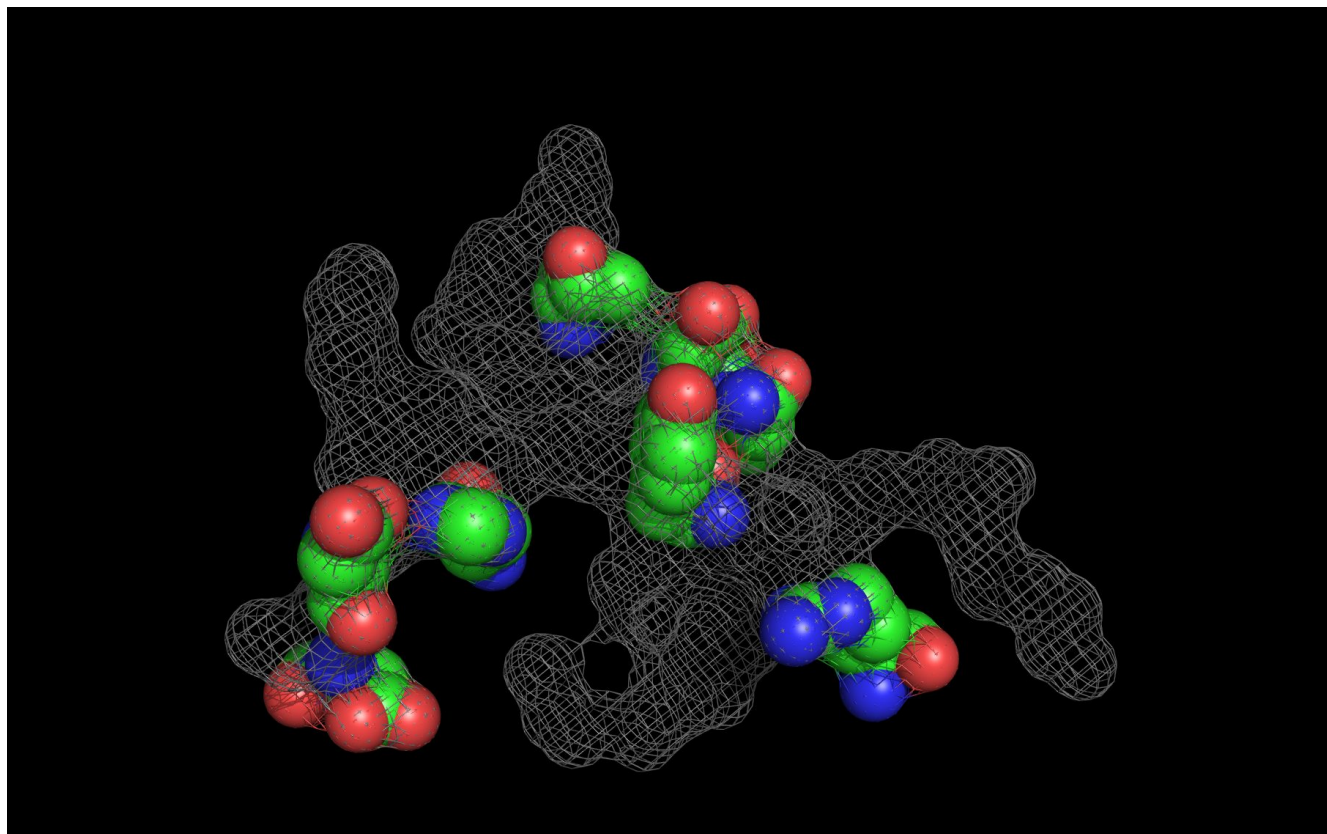
The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **Basiliximab residues contacting IL-2 charged atoms**

wwavePDB-identified basiliximab L chain residues ARG29, TYR31, ASP49, LYS52, SER91 and TYR93 and basiliximab H chain residues SER26, ARG29, TYR30, ASN53, ASP55, GLU63, ASP97, and TYR100 are shown contacting wwavePDB-identified IL2 charged atoms (antigen candidates) within the IL2 contact volume.

The grey surface encloses wwavePDB-identified contact atoms in residues from IL-2 that contact basiliximab. The spheres are color coded according to element (C N O).



### **IL-2 contact surface with residues contributing charged atoms**

The contacting atoms displayed in this example (and other more detailed information not included here) were delivered by Weininger Works™ wwavePDB in seconds using only the 3IU3.pdb<sup>1</sup> file as input.

***You don't have to be an antibody to know your antigen in seconds.***