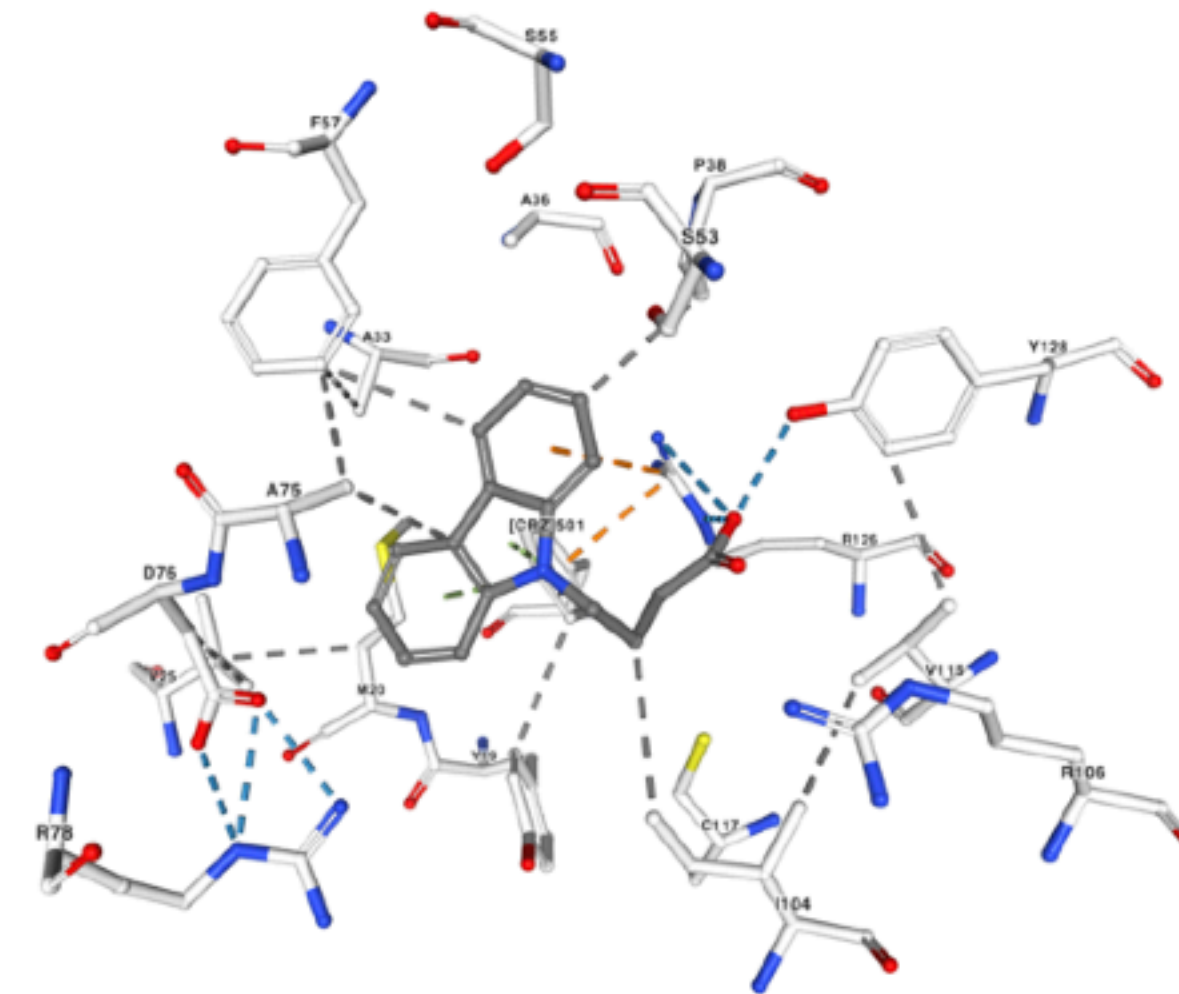


- For more drug-like interactions, see the ligand view for
- PDB ID 1TOW and Ligand [CRZ]501:A
- PDB ID 1PMN and Ligand [984]501:A

1TOW

Crystal structure of human adipocyte fatty acid binding protein in complex with a carboxylic acid ligand

Note: Use your mouse to drag, rotate, and zoom in and out of the structure. Mouse-over to identify atoms and bonds. [Mouse controls documentation.](#)



Spin ? Center ? Fullscreen ? Screenshot ? Perspective Camera ? White background ? Focus ? 0

Display Files ? Download Files ?

Structure View
Electron Density Maps
Ligand View

[Ligand View Documentation](#)

The ligand pocket is only visible if the opacity is set to greater than zero.

Ligand ? [CRZ]501:A ?

Pocket

Opacity ?

Near Clipping ?

Radius Clipping ?

Color ? By Hydrophobicity ?

Hydrogen Bonds (blue) ? ☒

Halogen Bonds (turquoise) ? ☒

Hydrophobic Contacts (grey) ? ☒

Pi Interactions (orange, green) ? ☒

Metal Interactions (purple) ? ☒

Label ? ☒

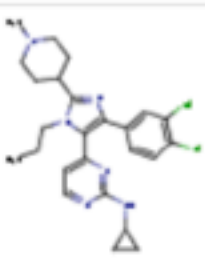
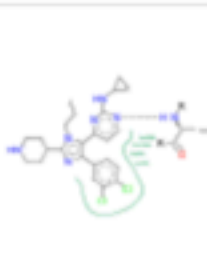
Polymer Display ? ☐



Default Ligand View ?

- A 3D Ligand View can sometimes look messy.
- Under the “Structure Summary” for a PDB entry, scroll down to “Small Molecules” and click on the right panel of “2D Diagram & Interactions”. This creates a Poseview Image, which more clearly shows which parts of the ligand interact with which amino acids in the protein.

Small Molecules

Ligands 1 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
984 Query on 984	A	CYCLOPROPYL-[4-[5-(3,4-DICHLOROPHENYL)-2-[(1-METHYL)-PIPERIDIN]-4-YL-3-PROPYL-3H-IMIDAZOL-4-YL]-PYRIMIDIN-2-YL]AMINE C ₂₅ H ₃₀ Cl ₂ N ₆ XCTKFTOEAKJMII-UHFFFAOYSA-N	 	Ligand Interaction

Download SDF File 
Download CCD File 

External Ligand Annotations

ID	Binding Affinity (Sequence Identity %)
984	IC50: 1.6 - 7.1 nM (100) BINDINGDB
984	IC50: 7.1 nM BINDINGMOAD
984	IC50: 7.1 nM PDBBIND

