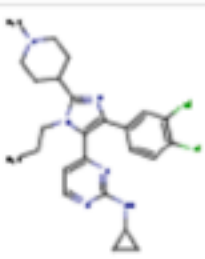
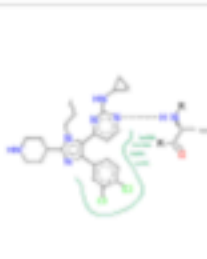




- A 3D Ligand View can sometimes look messy.
- Under the “Structure Summary” for a PDB entry, scroll down to “Small Molecules” and click on the right panel of “2D Diagram & Interactions”. This creates a Poseview Image, which more clearly shows which parts of the ligand interact with which amino acids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

Experimental Data & Validation

Experimental Data

Method: X-R
Resolution: 2
R-Value Free
R-Value Work
Space Group



Structure Validation

MyPDB

Small Molecules

Ligands 1 Unique

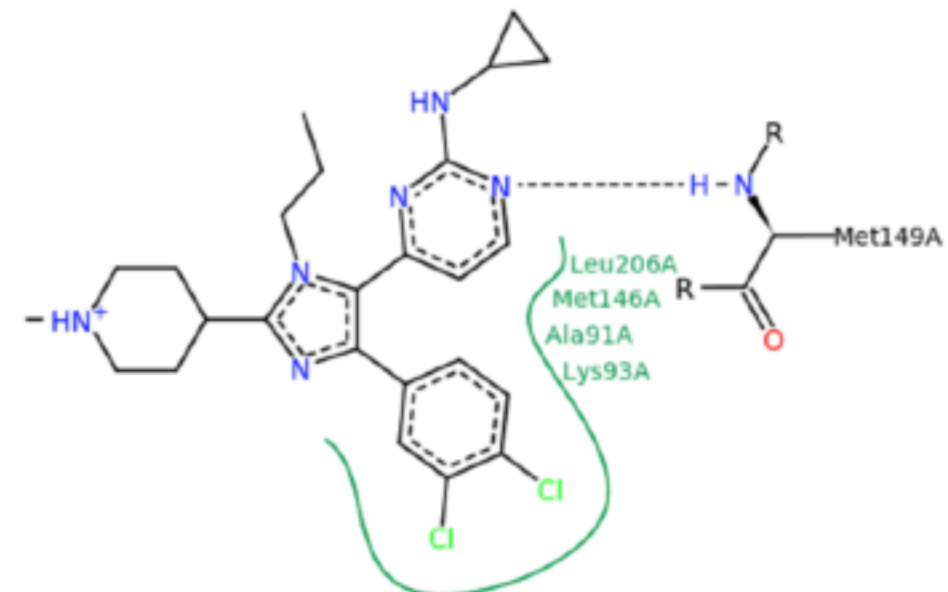
ID	Chains
984 Query on 984	A

Download SDF File 
Download CCD File 

External Ligand Annotations

ID	Binding A
984	IC50: 1.6
984	IC50: 7.1
984	IC50: 7.1

Poseview Image of 984 in 1PMN



3D Interactions

[Ligand Interaction](#)

