

Table 15S

The interactions of the H₂BT ligand, its complexes and DRO ligand with 2w3l target

Compound	ΔG_{bind} (kcal/mol)	Interaction(s)				Distance (Å)
		From	To	Category	Type	
H₂BT ligand	-4.08	6-ring	PHE63	Hydrophobic	Pi-Pi T-shaped	4.968
		6-ring	MET74		Pi-Alkyl	5.44
		6-ring	MET74			4.59
		6-ring	ARG105			4.96
		6-ring	ALA108			4.55
Co²⁺ complex	-4.11	NH	ASP70	H-Bond	Conventional H-Bond	2.32
		6-ring	VAL92	Hydrophobic	Pi-Alkyl	5.40
			LEU96			4.59
			ALA108			4.30
Ni²⁺ complex	-5.51	MET74	5-ring	Hydrophobic	Pi-Sigma	3.62
		MET74	6-ring			3.45
		6-ring	ALA108		Pi-Alkyl	4.33
		GLU73	6-ring		Amide-Pi Stacked	4.64
Cu²⁺ complex	-6.89	OH	PHE71	H-Bond	Pi-Donor H-Bond	2.52
		MET74	6-ring	Hydrophobic	Pi-Sigma	3.73
		GLU73	6-ring		Amide-Pi Stacked	4.72
		6-ring	ALA108		Pi-Alkyl	4.08
	-5.32	MET74	6-ring	H-Bond	Pi-Sigma	2.93

DRO ligand	LEU96	5-ring		3.73
	6-ring	PHE71	Pi-Pi T- Shaped	5.06
	6-ring	MET74		5.16
	6-ring	ALA108		5.01
	6-ring	VAL92		5.11
	6-ring	ARG105		5.43
	6-ring	ALA108		3.95
	6-ring	MET74		5.13