INTERACTION TABLE

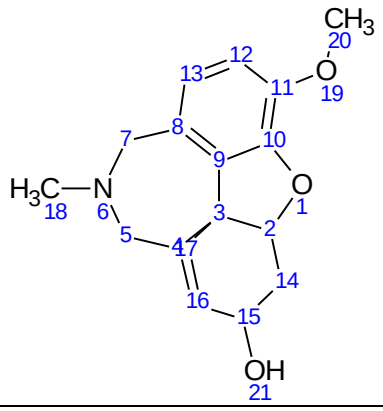
This example is for the galanthamine hetero compound complexed with 1DX6 protein. The ligplot was shown in an earlier document, and is also shown on the next page.

The Lewis structure for galanthamine was generated in ChemSketch from the SMILES notation found for the heterocompound on the RSPDB site. The numbering was automatically generated in ChemSketch.

"**HBD**" is a hydrogen-bond donor – this species has the H that is attached to an electronegative atom.
"**HBA**" is a hydrogen-bond acceptor – this electronegative atom is attracted to the H.
"**side chain**" means the protein interacts using the R group of the amino acid residue
"**backbone**" means the protein interacts using part of its peptide bond, and not the side chain atoms. The peptide bond will interact as either a HBD (H-N of peptide bond) or a HBA (O=C of peptide bond).
The numbers refer to the Lewis structure of the hetero compound.

Note: Most of the above interactions are visible only by rotating and inspecting the model in DSVisualizer.

Galanthamine (GNT)



Amino acid residue		*Hetero compound atoms*	*Nature of interaction*
asp 72	side chain is neg. charged carboxylate	??	doesn't seem to be in close contact – no H-bonds from H-bond monitor to near-by residues. Might be interaction with other hetero PG41.
trp 84	side chain – aromatic indole ring	hydrocarbon ring (2,3,14-17)	hydrophobic (the face of the trp indole ring is parallel to one of the hetero compound hydrocarbon rings
gly 117, 118, 119	side chain – H's	multi-rings	hydrophobic (the three gly residues, 117-119, are aligned near the face of the hetero compound's hydrocarbon rings)

glu 199	side chain	HO- (21)	residue carboxylate is the HBA; HO of hetero is HBD
ser 200	side chain -- -CH_2OH	CH_3-O-C (11,19,20)	ser is HBD; ether O of hetero is HBA
tyr 121	side chain –CH_2Ph-OH	????	tyr 121 doesn't seem to be in close contact with any hetero compound, or maybe an O on the PG4 1
phe 288, 290, 330, 331	side chain –CH_2Ph	aromatic ring (8-13)	the four phe residues, 288, 290, 330, 331, are either hydrophobic or edge-to-face stacked with the hetero aromatic ring
his 440	side chain	?	difficult to discern. Might be HBD to O in 5-membered hetero ring (HBA).