Most drug-target interactions are noncovalent

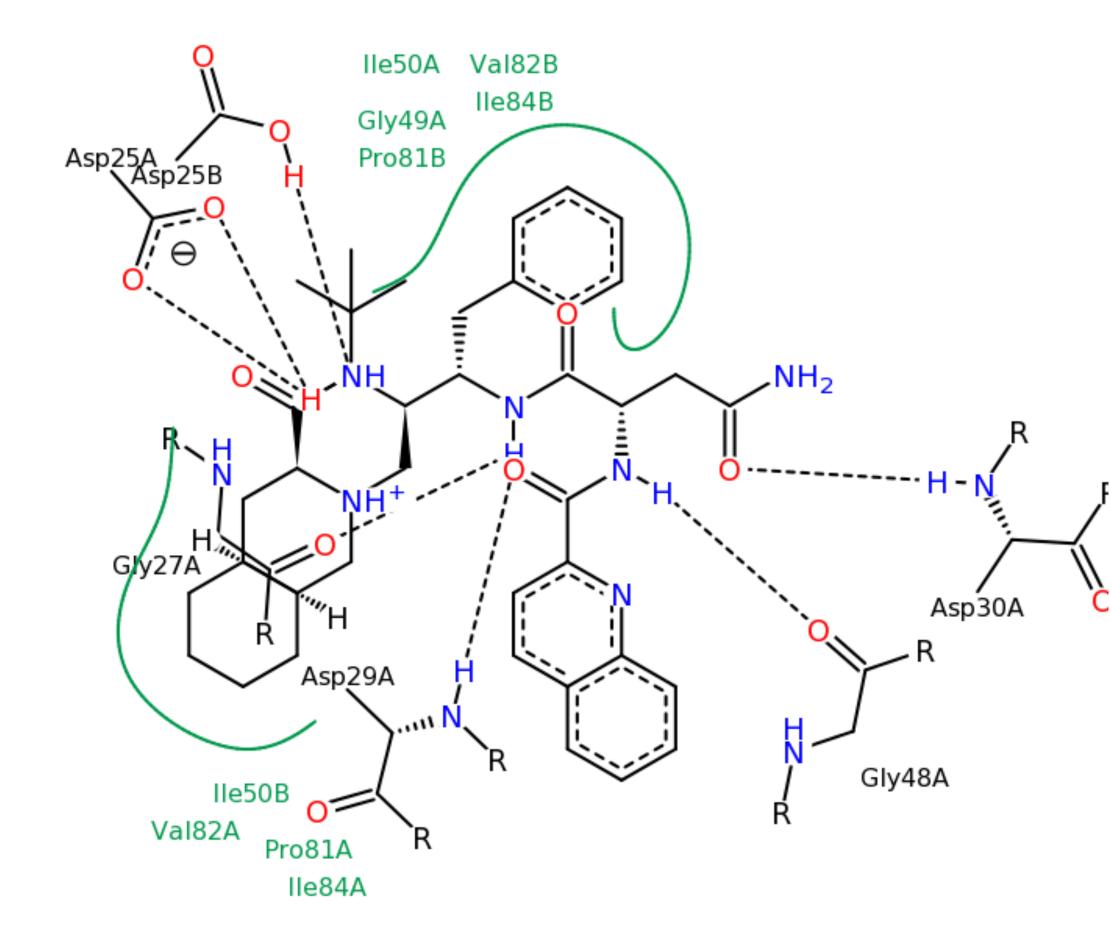
are primarily steric - van der Waals, atoms like to be close but not too close. electrostatic - like charges repel and opposite charges attract. H bonding

The interactions driving drug binding

often treated as electrostatic.

Water can play an important role.

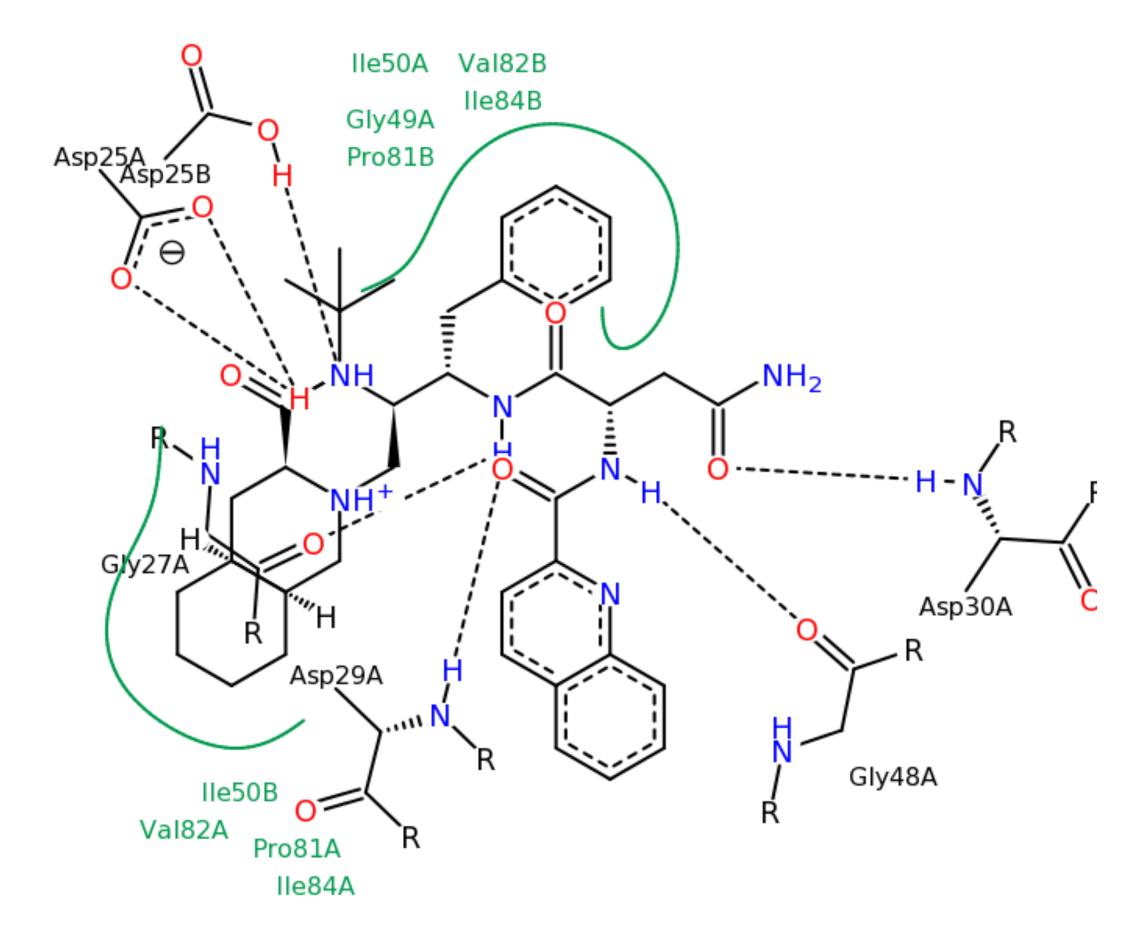
 Some drugs (like penicillin) bind to their targets covalently.



http://www.rcsb.org/pdb/101/motm_disscussed_entry.do?id=1hxb

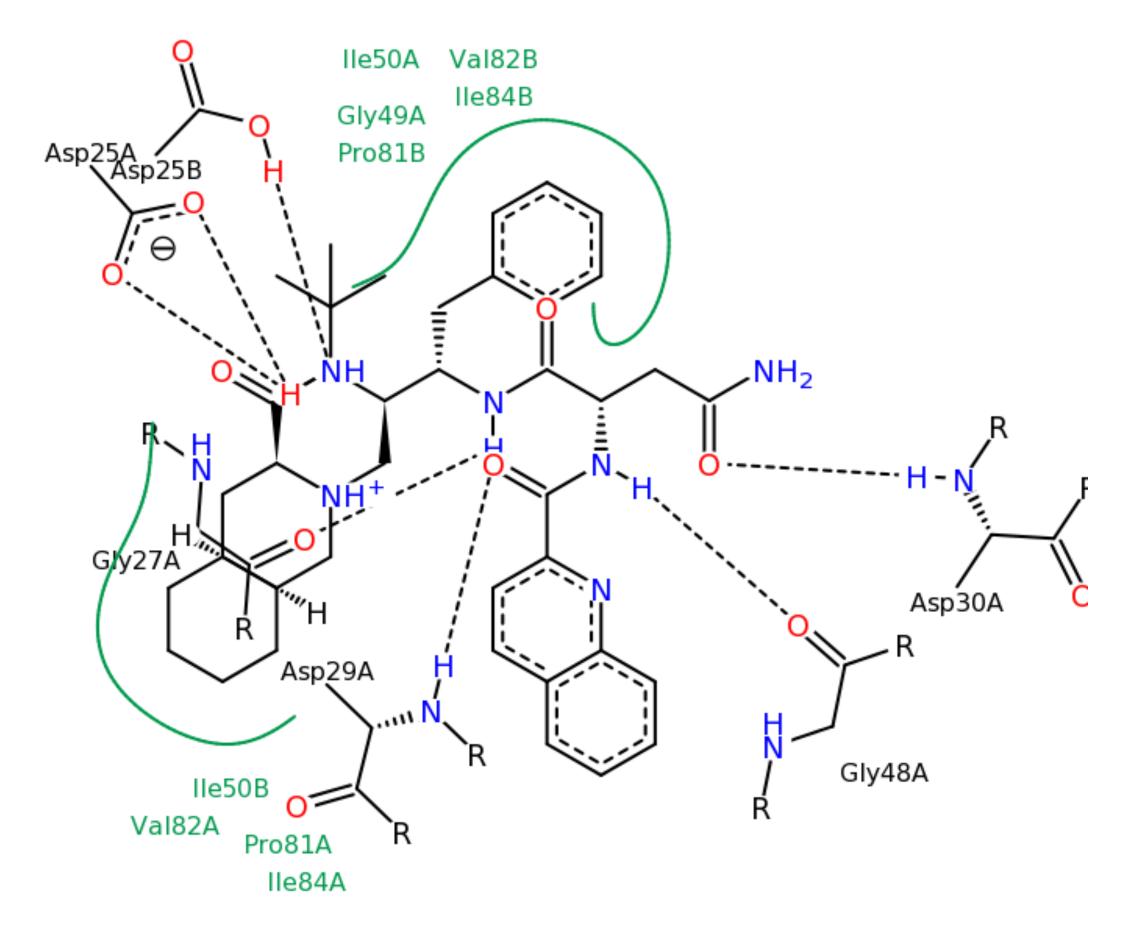
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 - electrostatic like charges repel and opposite charges attract. H bonding often treated as electrostatic.
- Water can play an important role.
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Drugs can be designed to optimize interactions



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