



- |  |                   |  |                    |  |                   |
|--|-------------------|--|--------------------|--|-------------------|
|  | polar             |  | sidechain acceptor |  | solvent residue   |
|  | acidic            |  | sidechain donor    |  | metal complex     |
|  | basic             |  | backbone acceptor  |  | solvent contact   |
|  | greasy            |  | backbone donor     |  | metal contact     |
|  | proximity contour |  | ligand exposure    |  | receptor exposure |