

Acid-base catalysis

Glu +1.0

His +1.0

Cys +1.0

Asp

Tyr

Ser

Lys

Thr



+0.5 per amino acid, up to +1.0

1 wrong amino acid: -0.25
2 wrong amino acids: -0.5
3 wrong amino acids: -0.75
4 wrong amino acids: -1.0
5 wrong amino acids: -1.25
6 wrong amino acids: -1.5

Side-chain functionalities have **pKa values** in (or near) the physiological pH range (+0.5), so they can be **{deprotonated/protonated or ionized}** (+0.5) sufficiently to act as **bases/acids** (+0.5) and, therefore, facilitate **nucleophilic** reactions (+0.5).

Those with pKa values slightly outside the physiological pH range can be “tuned” by their protein environment to have pKa values shifted into the physiological range. **Bonus +1.0**

*If you included Arg on your list, no marks will be deducted. For more details about Arg, please refer to the paper, Understanding the Functional Roles of Amino Acid Residues in Enzyme Catalysis, which was also posted on Piazza (<https://pubmed.ncbi.nlm.nih.gov/19447117/>)

Covalent catalysis

Cys +1.0

Ser +1.0

Lys

Asp

Thr

Tyr

His



+0.5 per amino acid, up to +1.0

1 wrong amino acid: -0.25
2 wrong amino acids: -0.5
3 wrong amino acids: -0.75
4 wrong amino acids: -1.0
5 wrong amino acids: -1.25
6 wrong amino acids: -1.5

Side-chain functionalities are {nucleophiles or have lone pairs of electrons} (+0.5) that can {attack electrophilic centres or make covalent bonds with the substrate} (+0.5).