**Table S1. Common ligand-amino acid and ligand-water molecule interactions**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligand 1(A201) | Interacting atoms | Distance (Å) | Ligand 2(B202) | Interacting atoms | Distance (Å) | Ligand 3(B203) | Interactingatoms | Distance (Å) |
| A201\_O2 | A113\_GLY\_N | 3.08 |  | B202\_O2 | B113\_GLY\_N | 3.12 |  | B203\_O2 | C113\_GLY\_N | 3.18 |
| A201\_O4 | A102\_GLY\_N | 2.85 |  | B202\_O4 | B102\_GLY\_N | 2.90 |  | B203\_O4 | C102\_GLY\_N | 2.84 |
| A201\_O4 | A308\_HOH\_O | 2.79 |  | B202\_O4 | B301\_HOH\_O | 2.80 |  | B203\_O4 | B303\_HOH\_O | 2.79 |
| A201\_N3 | A113\_GLY\_O | 2.80 |  | B202\_N3 | B113\_GLY\_O | 2.78 |  | B203\_N3 | C113\_GLY\_O | 2.81 |
| A201\_O3' | A105\_ASP\_OD2 | 2.83 |  | B202\_O3' | B105\_ASP\_OD2 | 2.66 |  | B203\_O3' | C105\_ASP\_OD2 | 2.65 |
| A201\_O3' | A105\_ASP\_N | 3.05 |  | B202\_O3' | B105\_ASP\_N | 3.19 |  | B203\_O3' | C105\_ASP\_N | 3.10 |
| A201\_O1A | B134\_GLN\_NE2 | 2.97 |  | B202\_O1A | C134\_GLN\_NE2 | 2.88 |  | B203\_O2A | A134\_GLN\_NE2 | 2.65 |
| A201\_O1A | A303\_HOH\_O | 2.73 |  | B202\_O1A | B505\_HOH\_O | 2.82 |  | B203\_O2A | B307\_HOH\_O | 2.64 |
| A201\_O2A | B134\_GLN\_NE2 | 3.00 |  | B202\_O2A | C134\_GLN\_NE2 | 2.90 |  | B203\_O2A | A134\_GLN\_NE2 | 2.60 |
| A201\_O2A | A449\_HOH\_O | 2.90 |  | B202\_O2A | B382\_HOH\_O | 2.71 |  | B203\_O1A | B349\_HOH\_O | 2.77 |
| A201\_O2A | B463\_HOH\_O | 2.86 |  | B202\_O2A | B408\_HOH\_O | 2.82 |  | B203\_O1A | A323\_HOH\_O | 2.86 |
| A201\_O2A | A447\_HOH\_O | 2.80 |  | B202\_O2A | B464\_HOH\_O | 2.76 |  | B203\_O1A | B405\_HOH\_O | 2.78 |
| A201\_N3A | B89\_SER\_OG | 2.57 |  | B202\_N3A | C89\_SER\_OG | 2.41 |  | B203\_N3A | A89\_SER\_OG | 2.75 |
| A201\_O1B | B90\_GLY\_N | 2.89 |  | B202\_O1B | C90\_GLY\_N | 2.94 |  | B203\_O2B | A90\_GLY\_N | 2.87 |
| A201\_O1B | A318\_HOH\_O | 2.68 |  | B202\_O1B | B325\_HOH\_O | 2.83 |  | B203\_O2B | B320\_HOH\_O | 2.60 |
| A201\_O2B | B88\_ARG\_NE | 2.83 |  | B202\_O2B | C88\_ARG\_NE | 2.85 |  | B203\_O1B | A88\_ARG\_NE | 2.77 |
| A201\_O2B | B88\_ARG\_NH2 | 3.06 |  | B202\_O2B | C88\_ARG\_NH2 | 2.98 |  | B203\_O1B | A88\_ARG\_NH2 | 3.02 |
| A201\_O2B | B366\_HOH\_O | 3.00 |  | B202\_O2B | C339\_HOH\_O | 3.05 |  | B203\_O1B | A393\_HOH\_O | 3.07 |
| A201\_O2B | B463\_HOH\_O | 2.91 |  | B202\_O2B | B408\_HOH\_O | 2.95 |  | B203\_O1B | A323\_HOH\_O | 2.94 |
| A201\_O1G | B366\_HOH\_O | 2.87 |  | B202\_O1G | C339\_HOH\_O | 2.91 |  | B203\_O1G | A393\_HOH\_O | 2.87 |
| A201\_O1G | A447\_HOH\_O | 2.86 |  | B202\_O1G | B464\_HOH\_O | 3.01 |  | B203\_O1G | B405\_HOH\_O | 3.07 |

**Table B. Common water-amino acid interactions at active site**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligand 1 water | Interacting atoms | Distance (Å) | Ligand 2water | InteractingAtoms | Distance (Å) | Ligand 3water | Interacting Atoms | Distance (Å) |
| A308\_HOH\_O | A100\_GLY\_O | 2.83 |  | B301\_HOH\_O | B100\_GLY\_O | 2.86 |  | B303\_HOH\_O | C100\_GLY\_O | 2.88 |
| A303\_HOH\_O | B87\_PRO\_O | 2.86 |  | B505\_HOH\_O | C87\_PRO\_O | 2.88 |  | B307\_HOH\_O | A87\_PRO\_O | 2.91 |
| A303\_HOH\_O | A103\_VAL\_N | 3.04 |  | B505\_HOH\_O | B103\_VAL\_N | 3.03 |  | B307\_HOH\_O | C103\_VAL\_N | 2.98 |
| A449\_HOH\_O | A105\_ASP\_OD2 | 2.86 |  | B382\_HOH\_O | B105\_ASP\_OD2 | 2.95 |  | B349\_HOH\_O | C105\_ASP\_OD2 | 2.85 |
| A449\_HOH\_O | A105\_ASP\_OD1 | 2.97 |  | B382\_HOH\_O | B105\_ASP\_OD1 | 3.30 |  | B349\_HOH\_O | C105\_ASP\_OD1 | 2.94 |
| B341\_HOH\_O | A105\_ASP\_OD1 | 2.86 |  | B343\_HOH\_O | B105\_ASP\_OD1 | 2.60 |  | C337\_HOH\_O | C105\_ASP\_OD1 | 2.60 |
| A308\_HOH\_O | A115\_ILE\_N | 2.86 |  | B301\_HOH\_O | B115\_ILE\_N | 2.84 |  | B303\_HOH\_O | C115\_ILE\_N | 2.84 |
| B463\_HOH\_O | B134\_GLN\_OE1 | 2.90 |  | B408\_HOH\_O | C134\_GLN\_OE1 | 2.90 |  | A323\_HOH\_O | A134\_GLN\_OE1 | 2.86 |
| B366\_HOH\_O | B52\_ASP\_OD2 | 2.60 |  | C339\_HOH\_O | C52\_ASP\_OD2 | 2.71 |  | A393\_HOH\_O | A52\_ASP\_OD2 | 2.74 |
| B463\_HOH\_O | B52\_ASP\_OD1 | 2.65 |  | B408\_HOH\_O | C52\_ASP\_OD1 | 2.84 |  | A323\_HOH\_O | A52\_ASP\_OD1 | 2.68 |
| B463\_HOH\_O | B134\_GLN\_OE1 | 2.90 |  | B408\_HOH\_O | C134\_GLN\_OE1 | 3.14 |  | A323\_HOH\_O | A134\_GLN\_OE1 | 2.90 |
| A318\_HOH\_O | B91\_LEU\_N | 2.90 |  | B325\_HOH\_O | C91\_LEU\_N | 3.00 |  | B320\_HOH\_O | A91\_LEU\_N | 2.90 |
| A449\_HOH\_O | B134\_GLN\_OE1 | 3.20 |  | B382\_HOH\_O | C134\_GLN\_OE1 | 3.20 |  | B349\_HOH\_O | A134\_GLN\_OE1 | 3.02 |
| A449\_HOH\_O | A103\_VAL\_O | 3.16 |  | B382\_HOH\_O | B103\_VAL\_O | 3.20 |  | B349\_HOH\_O | C103\_VAL\_O | 3.13 |

Ligands are referred by their chain ID and residue numbers used in the PDB file. Atoms interacting with ligands are indicated by the following description; chain ID, residue number, residue name, and interacting atom name. The distances were obtained by COOT. The underlined water molecules are ones directly interacting with magnesium ions at the active sites. Gray highlighted water molecules are catalytic water molecules.