Metal Complexes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Metal | Target | Distance | Location |
| Complex 1: Cu, trigonal.planar (3) |
| 1 | 46A | HIS | 2411 | 367 | 1.99 | protein.sidechain |
| 2 | 48A | HIS | 2411 | 387 | 1.96 | protein.sidechain |
| 3 | 120A | HIS | 2411 | 945 | 2.02 | protein.sidechain |

Metal Complexes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Metal | Target | Distance | Location |
| Complex 1: Cu, trigonal.planar (3) |
| 1 | 46F | HIS | 2425 | 1570 | 2.00 | protein.sidechain |
| 2 | 48F | HIS | 2425 | 1590 | 1.94 | protein.sidechain |
| 3 | 120F | HIS | 2425 | 2160 | 2.02 | protein.sidechain |

Metal Complexes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Metal | Target | Distance | Location |
| Complex 1: Zn, trigonal.bipyramidal (5) |
| 1 | 63A | HIS | 2413 | 490 | 2.01 | protein.sidechain |
| 2 | 71A | HIS | 2413 | 560 | 1.97 | protein.sidechain |
| 3 | 80A | HIS | 2413 | 637 | 2.01 | protein.sidechain |
| 4 | 83A | ASP | 2413 | 658 | 1.93 | protein.sidechain |
| 5 | 83A | ASP | 2413 | 659 | 2.85 | protein.sidechain |

Metal Complexes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Metal | Target | Distance | Location |
| Complex 1: Zn, trigonal.bipyramidal (5) |
| 1 | 63F | HIS | 2427 | 1693 | 1.99 | protein.sidechain |
| 2 | 71F | HIS | 2427 | 1766 | 2.02 | protein.sidechain |
| 3 | 80F | HIS | 2427 | 1843 | 2.00 | protein.sidechain |
| 4 | 83F | ASP | 2427 | 1864 | 1.92 | protein.sidechain |
| 5 | 83F | ASP | 2427 | 1865 | 2.84 | protein.sidechain |

Hydrogen Bonds

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Distance H-A | Distance D-A | Donor Angle | Protein donor? | Side chain | Donor Atom | Acceptor Atom |
| 1 | 137A | THR | 2.50 | 2.87 | 102.56 |  |  | 2415 [O3] | 1078 [O3] |
| 2 | 141A | GLY | 2.13 | 2.90 | 133.78 |  |  | 1097 [Nam] | 2416 [O3] |

Hydrogen Bonds

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Distance H-A | Distance D-A | Donor Angle | Protein donor? | Side chain | Donor Atom | Acceptor Atom |
| 1 | 58A | THR | 3.21 | 3.92 | 131.01 |  |  | 2420 [O3] | 460 [O3] |
| 2 | 143A | ARG | 1.87 | 2.84 | 169.44 |  |  | 1108 [Nam] | 2423 [O3] |

Water Bridges

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Dist. A-W | Dist. D-W | Donor Angle | Water Angle | Protein donor? | Donor Atom | Acceptor Atom | Water Atom |
| 1 | 58A | THR | 3.74 | 4.09 | 156.25 | 108.25 |  | 2421 [O3] | 460 [O3] | 2567 |
| 2 | 58A | THR | 4.09 | 3.74 | 140.29 | 101.68 |  | 460 [O3] | 2421 [O3] | 2567 |
| 3 | 58A | THR | 2.58 | 3.23 | 136.48 | 71.62 |  | 2421 [O3] | 460 [O3] | 2570 |
| 4 | 143A | ARG | 3.44 | 3.86 | 118.54 | 93.81 |  | 2422 [O3] | 1115 [Ng+] | 2733 |

Hydrogen Bonds

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Distance H-A | Distance D-A | Donor Angle | Protein donor? | Side chain | Donor Atom | Acceptor Atom |
| 1 | 141F | GLY | 2.78 | 3.47 | 128.51 |  |  | 2324 [Nam] | 2432 [O3] |

Water Bridges

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Dist. A-W | Dist. D-W | Donor Angle | Water Angle | Protein donor? | Donor Atom | Acceptor Atom | Water Atom |
| 1 | 139F | ASN | 2.81 | 2.81 | 158.84 | 80.63 |  | 2318 [Nam] | 2432 [O3] | 3011 |
| 2 | 139F | ASN | 3.09 | 2.71 | 118.95 | 93.75 |  | 2318 [Nam] | 2432 [O3] | 3032 |
| 3 | 139F | ASN | 2.92 | 2.71 | 118.95 | 83.89 |  | 2318 [Nam] | 2436 [O3] | 3032 |
| 4 | 141F | GLY | 2.81 | 2.76 | 106.74 | 98.48 |  | 2430 [O3] | 2327 [O2] | 3035 |

Hydrogen Bonds

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Distance H-A | Distance D-A | Donor Angle | Protein donor? | Side chain | Donor Atom | Acceptor Atom |
| 1 | 143F | ARG | 1.94 | 2.91 | 165.36 |  |  | 2334 [Nam] | 2440 [O3] |

Water Bridges

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Dist. A-W | Dist. D-W | Donor Angle | Water Angle | Protein donor? | Donor Atom | Acceptor Atom | Water Atom |
| 1 | 141F | GLY | 3.11 | 2.93 | 122.06 | 94.55 |  | 2442 [O3] | 2327 [O2] | 3041 |
| 2 | 142F | SER | 3.79 | 2.87 | 101.61 | 84.77 |  | 2333 [O3] | 2440 [O3] | 3012 |
| 3 | 143F | ARG | 3.11 | 2.93 | 122.06 | 87.41 |  | 2442 [O3] | 2341 [Ng+] | 3041 |

Hydrogen Bonds

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Index | Residue | AA | Distance H-A | Distance D-A | Donor Angle | Protein donor? | Side chain | Donor Atom | Acceptor Atom |
| 1 | 131A | ASN | 2.45 | 3.08 | 119.55 |  |  | 1031 [N3] | 2447 [O3] |
| 2 | 132A | GLU | 2.32 | 2.77 | 106.82 |  |  | 1033 [Nam] | 2447 [O3] |
| 3 | 133A | GLU | 1.80 | 2.78 | 169.10 |  |  | 1042 [Nam] | 2447 [O3] |