**Supplementary Data S6:** *Contact residues of EcoTrx1 and HsTrx1 in their crystal complexes with protein ligands*

# Distinct or shared areas of mitochondrial thioredoxin 2 may be used for its covalent and strong non-covalent interactions with protein ligands

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**1. Contact residues of EcoTrx1 in its crystal complexes with protein ligands**

**1.1. T7 DNA polymerase (PDB ID: 1T7P): a complex of EcoTrx1 with G5p** [1].

| Interacting residues (G5p-EcoTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| G5p:THR327:N - EcoTrx1:ILE75:O | Hydrogen Bond (conventional) | G5p:THR327:N (H-donor) | EcoTrx1:ILE75:O (H-acceptor) | 2.90286 |
| G5p:THR327:OG1 - EcoTrx1:CYS32:SG | Hydrogen Bond (conventional) | G5p:THR327:OG1 (H-donor) | EcoTrx1:CYS32:SG (H-acceptor) | 2.994 |
| G5p:VAL329:N - EcoTrx1:ARG73:O | Hydrogen Bond (conventional) | G5p:VAL329:N (H-donor) | EcoTrx1:ARG73:O (H-acceptor) | 3.0883 |
| EcoTrx1:ARG73:NH2 - G5p:TYR320:OH | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NH2 (H-donor) | G5p:TYR320:OH (H-acceptor) | 2.86865 |
| EcoTrx1:ARG73:NH2 - G5p:TYR326:OH | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NH2 (H-donor) | G5p:TYR326:OH (H-acceptor) | 3.28787 |
| EcoTrx1:ILE75:N - G5p:THR327:O | Hydrogen Bond (conventional) | EcoTrx1:ILE75:N (H-donor) | G5p:THR327:O (H-acceptor) | 3.02215 |
| EcoTrx1:THR89:OG1 - G5p:GLU319:OE1 | Hydrogen Bond (conventional) | EcoTrx1:THR89:OG1 (H-donor) | G5p:GLU319:OE1 (H-acceptor) | 3.10654 |
| EcoTrx1:VAL91:N - G5p:GLU319:O | Hydrogen Bond (conventional) | EcoTrx1:VAL91:N (H-donor) | G5p:GLU319:O (H-acceptor) | 2.92813 |
| EcoTrx1:ALA93:N - G5p:PRO325:O | Hydrogen Bond (conventional) | EcoTrx1:ALA93:N (H-donor) | G5p:PRO325:O (H-acceptor) | 2.78199 |
| G5p:PRO287:CD - EcoTrx1:TRP31:O | Hydrogen Bond (carbon) | G5p:PRO287:CD (H-donor) | EcoTrx1:TRP31:O (H-acceptor) | 3.08175 |
| EcoTrx1:PRO34:CD - G5p:THR327:OG1 | Hydrogen Bond (carbon) | EcoTrx1:PRO34:CD (H-donor) | G5p:THR327:OG1 (H-acceptor) | 3.47822 |
| G5p:PRO277 - EcoTrx1:MET37 | Hydrophobic (alkyl) | G5p:PRO277 (alkyl) | EcoTrx1:MET37 (alkyl) | 4.81137 |
| G5p:VAL321 - EcoTrx1:LEU94 | Hydrophobic (alkyl) | G5p:VAL321 (alkyl) | EcoTrx1:LEU94 (alkyl) | 4.75678 |
| G5p:ALA324 - EcoTrx1:LEU94 | Hydrophobic (alkyl) | G5p:ALA324 (alkyl) | EcoTrx1:LEU94 (alkyl) | 4.65972 |
| G5p:PRO325 - EcoTrx1:PRO34 | Hydrophobic (alkyl) | G5p:PRO325 (alkyl) | EcoTrx1:PRO34 (alkyl) | 5.03292 |
| G5p:VAL329 - EcoTrx1:ILE75 | Hydrophobic (alkyl) | G5p:VAL329 (alkyl) | EcoTrx1:ILE75 (alkyl) | 4.66883 |
| EcoTrx1:PRO34 - G5p:ILE289 | Hydrophobic (alkyl) | EcoTrx1:PRO34 (alkyl) | G5p:ILE289 (alkyl) | 5.28245 |
| EcoTrx1:ALA93 - G5p:PRO325 | Hydrophobic (alkyl) | EcoTrx1:ALA93 (alkyl) | G5p:PRO325 (alkyl) | 4.38959 |
| G5p:TYR265 - EcoTrx1:ILE60 | Hydrophobic (Pi-alkyl) | G5p:TYR265 (Pi-orbitals) | EcoTrx1:ILE60 (alkyl) | 5.12054 |
| G5p:TYR265 - EcoTrx1:ALA67 | Hydrophobic (Pi-alkyl) | G5p:TYR265 (Pi-orbitals) | EcoTrx1:ALA67 (alkyl) | 4.67645 |
| G5p:TYR265 - EcoTrx1:PRO68 | Hydrophobic (Pi-alkyl) | G5p:TYR265 (Pi-orbitals) | EcoTrx1:PRO68 (alkyl) | 5.38793 |
| G5p:PHE274 - EcoTrx1:PRO34 | Hydrophobic (Pi-alkyl) | G5p:PHE274 (Pi-orbitals) | EcoTrx1:PRO34 (alkyl) | 5.30569 |

| | | | | |
|---|---|---|---|---|
| G5p:TYR320 - EcoTrx1:VAL91 | Hydrophobic (Pi-alkyl) | G5p:TYR320 (Pi-orbitals) | EcoTrx1:VAL91 (alkyl) | 4.82123 |
| G5p:TYR326 - EcoTrx1:VAL91 | Hydrophobic (Pi-alkyl) | G5p:TYR326 (Pi-orbitals) | EcoTrx1:VAL91 (alkyl) | 5.40115 |
| G5p:HIS331 - EcoTrx1:PRO68 | Hydrophobic (Pi-alkyl) | G5p:HIS331 (Pi-orbitals) | EcoTrx1:PRO68 (alkyl) | 4.30139 |
| EcoTrx1:TRP31 - G5p:PRO267 | Hydrophobic (Pi-alkyl) | EcoTrx1:TRP31 (Pi-orbitals) | G5p:PRO267 (alkyl) | 4.95059 |
| EcoTrx1:MET37:SD - G5p:PHE274 | Other (Pi-sulfur) | EcoTrx1:MET37:SD (sulfur) | G5p:PHE274 (Pi-orbitals) | 5.19383 |

| EcoTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| TRP31 | - | + | - | + | - |
| CYS32 | - | + | - | - | - |
| PRO34 | - | + | - | + | - |
| MET37 | - | - | - | + | + |
| ILE60 | - | - | - | + | - |
| ALA67 | - | - | - | + | - |
| PRO68 | - | - | - | + | - |
| ARG73 | - | + | - | - | - |
| ILE75 | - | + | - | + | - |
| THR89 | - | + | - | - | - |
| VAL91 | - | + | - | + | - |
| ALA93 | - | + | - | + | - |
| LEU94 | - | - | - | + | - |

### 1.2. TrxR-EcoTrx1 complex (PDB: 1F6M) [2].

| Interacting residues (TrxR-EcoTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| TrxR:ARG130:NH2 – EcoTrx1:TYR70:O | Hydrogen Bond (conventional) | TrxR:ARG130:NH2 (H-donor) | EcoTrx1:TYR70:O (H-acceptor) | 2.60149 |
| EcoTrx1:TRP31:NE1 – TrxR:CYS138:O | Hydrogen Bond (conventional) | EcoTrx1:TRP31:NE1 (H-donor) | TrxR:CYS138:O (H-acceptor) | 3.13459 |
| EcoTrx1:ARG73:N – TrxR:GLY129:O | Hydrogen Bond (conventional) | EcoTrx1:ARG73:N (H-donor) | TrxR:GLY129:O (H-acceptor) | 3.25012 |
| EcoTrx1:ARG73:NE – TrxR:ARG130:O | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NE (H-donor) | TrxR:ARG130:O (H-acceptor) | 3.07444 |
| EcoTrx1:ARG73:NH1 – TrxR:ARG130:O | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NH1 (H-donor) | TrxR:ARG130:O (H-acceptor) | 2.85782 |
| EcoTrx1:ARG73:NH1 – TrxR:ALA237:O | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NH1 (H-donor) | TrxR:ALA237:O (H-acceptor) | 2.71026 |
| EcoTrx1:ILE75:N – TrxR:ASP139:OD1 | Hydrogen Bond (conventional) | EcoTrx1:ILE75:N (H-donor) | TrxR:ASP139:OD1 (H-acceptor) | 2.78878 |
| EcoTrx1:TRP31:CD1 – TrxR:THR137:O | Hydrogen Bond (carbon) | EcoTrx1:TRP31:CD1 (H-donor) | TrxR:THR137:O (H-acceptor) | 3.49543 |

| | | | | |
|---|---|---|---|---|
| EcoTrx1:ARG73:C.O;GLY74:N – TrxR:PHE142 | Hydrophobic (amide-Pi stacked) | EcoTrx1:ARG73:C.O;GLY74:N (amide) | TrxR:PHE142 (Pi-orbitals) | 3.91293 |
| TrxR:LYS39 – EcoTrx1:MET37 | Hydrophobic (alkyl) | TrxR:LYS39 (alkyl) | EcoTrx1:MET37 (alkyl) | 4.67061 |
| TrxR:CYS138 – EcoTrx1:PRO34 | Hydrophobic (alkyl) | TrxR:CYS138 (alkyl) | EcoTrx1:PRO34 (alkyl) | 5.06124 |
| TrxR:CYS138 – EcoTrx1:ILE75 | Hydrophobic (alkyl) | TrxR:CYS138 (alkyl) | EcoTrx1:ILE75 (alkyl) | 5.48344 |
| EcoTrx1:ALA93 – TrxR:MET37 | Hydrophobic (alkyl) | EcoTrx1:ALA93 (alkyl) | TrxR:MET37 (alkyl) | 4.57981 |
| TrxR:PHE81 – EcoTrx1:MET37 | Hydrophobic (Pi-alkyl) | TrxR:PHE81 (Pi-orbitals) | EcoTrx1:MET37 (alkyl) | 5.33256 |
| TrxR:PHE81 – EcoTrx1:PRO40 | Hydrophobic (Pi-alkyl) | TrxR:PHE81 (Pi-orbitals) | EcoTrx1:PRO40 (alkyl) | 5.46234 |
| TrxR:PHE142 – EcoTrx1:ARG73 | Hydrophobic (Pi-alkyl) | TrxR:PHE142 (Pi-orbitals) | EcoTrx1:ARG73 (alkyl) | 4.64594 |
| TrxR:PHE142 – EcoTrx1:ILE75 | Hydrophobic (Pi-alkyl) | TrxR:PHE142 (Pi-orbitals) | EcoTrx1:ILE75 (alkyl) | 5.44979 |
| TrxR:TYR143 – EcoTrx1:ARG73 | Hydrophobic (Pi-alkyl) | TrxR:TYR143 (Pi-orbitals) | EcoTrx1:ARG73 (alkyl) | 5.46537 |

| EcoTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| TRP31 | - | + | - | - | - |
| PRO34 | - | - | - | + | - |
| MET37 | - | - | - | + | - |
| PRO40 | - | - | - | + | - |
| TYR70 | - | + | - | - | - |
| ARG73 | - | + | - | + | - |
| ILE75 | - | + | - | + | - |
| ALA93 | - | - | - | + | - |

### 1.3. MsrA-EcoTrx1 (PDB: 6YEV).

| Interacting residues (MsrA-EcoTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| EcoTrx1:LYS90:NZ – MsrA:ASP164:OD2 | Electrostatic (Attractive Charge) | EcoTrx1:LYS90:NZ (Positive) | MsrA:ASP164:OD2 (Negative) | 5.5975 |
| EcoTrx1:ALA93:N – MsrA:GLY204:O | Hydrogen Bond (conventional) | EcoTrx1:ALA93:N (H-Donor) | MsrA:GLY204:O (H-Acceptor) | 2.83316 |
| MsrA:CYS206:N – EcoTrx1:ILE75:O | Hydrogen Bond (conventional) | MsrA:CYS206:N (H-Donor) | EcoTrx1:ILE75:O (H-Acceptor) | 3.00363 |
| EcoTrx1:PRO34:CD – MsrA:GLU116:OE2 | Hydrogen Bond (carbon) | EcoTrx1:PRO34:CD (H-Donor) | MsrA:GLU116:OE2 (H-Acceptor) | 3.73592 |
| MsrA:PRO208:CD – EcoTrx1:ARG73:O | Hydrogen Bond (carbon) | MsrA:PRO208:CD (H-Donor) | EcoTrx1:ARG73:O (H-Acceptor) | 3.29517 |
| MsrA:ALA162 – EcoTrx1:VAL91 | Hydrophobic (alkyl) | MsrA:ALA162 (Alkyl) | EcoTrx1:VAL91 (Alkyl) | 4.2169 |

| | | | | |
|---|---|---|---|---|
| MsrA:ALA163 – EcoTrx1:VAL91 | Hydrophobic (alkyl) | MsrA:ALA163 (Alkyl) | EcoTrx1:VAL91 (Alkyl) | 4.08484 |
| MsrA:CYS206 – EcoTrx1:PRO34 | Hydrophobic (alkyl) | MsrA:CYS206 (Alkyl) | EcoTrx1:PRO34 (Alkyl) | 4.83189 |
| MsrA:PRO208 – EcoTrx1:ILE75 | Hydrophobic (alkyl) | MsrA:PRO208 (Alkyl) | EcoTrx1:ILE75 (Alkyl) | 5.41164 |
| EcoTrx1:TRP31 – MsrA:CYS206 | Hydrophobic (Pi-alkyl) | EcoTrx1:TRP31 (Pi-Orbitals) | MsrA:CYS206 (Alkyl) | 5.10675 |

| EcoTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| TRP31 | | | | + | |
| PRO34 | | + | | + | |
| ARG73 | | + | | | |
| ILE75 | | + | | + | |
| LYS90 | + | | | | |
| VAL91 | | | | ++ | |
| ALA93 | | + | | | |

### 1.4. PAPS reductase-EcoTrx1 (PDB: 2O8V) [3].

| Interacting residues (MsrA-EcoTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| EcoTrx1:LYS36:NZ – PAPS red:ASP206:OD1 | Hydrogen Bond;Electrostatic (Salt Bridge) | EcoTrx1:LYS36:NZ (H-donor) | PAPS red:ASP206:OD1 (H-acceptor) | 2.82895 |
| EcoTrx1:ARG73:NH1 – PAPS red:GLU238:OE2 | Hydrogen Bond;Electrostatic (Salt Bridge) | EcoTrx1:ARG73:NH1 (H-donor) | PAPS red:GLU238:OE2 (H-acceptor) | 2.86245 |
| EcoTrx1:ARG73:NH2 – PAPS red:GLU243:OE2 | Hydrogen Bond;Electrostatic (Salt Bridge) | EcoTrx1:ARG73:NH2 (H-donor) | PAPS red:GLU243:OE2 (H-acceptor) | 2.6723 |
| EcoTrx1:ARG73:NH1 – PAPS red:GLU243:OE1 | Electrostatic (Attractive Charge) | EcoTrx1:ARG73:NH1 (positive) | PAPS red:GLU243:OE1 (negative) | 3.99202 |
| EcoTrx1:ARG73:NH2 – PAPS red:GLU238:OE1 | Electrostatic (Attractive Charge) | EcoTrx1:ARG73:NH2 (positive) | PAPS red:GLU238:OE1 (negative) | 2.97327 |
| PAPS red:TRP205:NE1 – EcoTrx1:GLU30:O | Hydrogen Bond (conventional) | PAPS red:TRP205:NE1 (H-donor) | EcoTrx1:GLU30:O (H-acceptor) | 2.95719 |
| PAPS red:CYS239:N – EcoTrx1:ILE75:O | Hydrogen Bond (conventional) | PAPS red:CYS239:N (H-donor) | EcoTrx1:ILE75:O (H-acceptor) | 3.05945 |
| PAPS red:LEU241:N – EcoTrx1:ARG73:O | Hydrogen Bond (conventional) | PAPS red:LEU241:N (H-donor) | EcoTrx1:ARG73:O (H-acceptor) | 3.38506 |
| EcoTrx1:LYS36:NZ – PAPS red:TRP205:O | Hydrogen Bond (conventional) | EcoTrx1:LYS36:NZ (H-donor) | PAPS red:TRP205:O (H-acceptor) | 3.28943 |
| EcoTrx1:ARG73:NE – PAPS red:GLU243:OE1 | Hydrogen Bond (conventional) | EcoTrx1:ARG73:NE (H-donor) | PAPS red:GLU243:OE1 | 2.73015 |

| | | | | |
|---|---|---|---|---|
| | | | (H-acceptor) | |
| EcoTrx1:ALA93:N – PAPS red:ARG237:O | Hydrogen Bond (conventional) | EcoTrx1:ALA93:N (H-donor) | PAPS red:ARG237:O (H-acceptor) | 2.85509 |
| EcoTrx1:LYS36:NZ – PAPS red:TRP205 | Electrostatic (Pi-Cation) | EcoTrx1:LYS36:NZ (positive) | PAPS red:TRP205 (Pi-orbitals) | 4.59989 |
| PAPS red:ASN187:C.O;ARG188:N – EcoTrx1:TRP31 | Hydrophobic (Amide-Pi Stacked) | PAPS red:ASN187:C.O;ARG188:N (amide) | EcoTrx1:TRP31 (Pi-orbitals) | 4.35499 |
| PAPS red:ASN187:C.O;ARG188:N – EcoTrx1:TRP31 | Hydrophobic (Amide-Pi Stacked) | PAPS red:ASN187:C.O;ARG188:N (amide) | EcoTrx1:TRP31 (Pi-orbitals) | 4.67411 |
| PAPS red:CYS239 – EcoTrx1:PRO34 | Hydrophobic (alkyl) | PAPS red:CYS239 (alkyl) | EcoTrx1:PRO34 (alkyl) | 4.8634 |
| PAPS red:LEU241 – EcoTrx1:ILE60 | Hydrophobic (alkyl) | PAPS red:LEU241 (alkyl) | EcoTrx1:ILE60 (alkyl) | 5.37286 |
| PAPS red:LEU241 – EcoTrx1:ILE75 | Hydrophobic (alkyl) | PAPS red:LEU241 (alkyl) | EcoTrx1:ILE75 (alkyl) | 5.02976 |
| EcoTrx1:PRO34 – PAPS red:LEU235 | Hydrophobic (alkyl) | EcoTrx1:PRO34 (alkyl) | PAPS red:LEU235 (alkyl) | 4.33625 |
| PAPS red:TRP205 – EcoTrx1:LYS36 | Hydrophobic (Pi-alkyl) | PAPS red:TRP205 (Pi-orbitals) | EcoTrx1:LYS36 (alkyl) | 5.14881 |
| PAPS red:TRP205 – EcoTrx1:LYS36 | Hydrophobic (Pi-alkyl) | PAPS red:TRP205 (Pi-orbitals) | EcoTrx1:LYS36 (alkyl) | 5.16558 |
| EcoTrx1:TRP31 – PAPS red:ARG188 | Hydrophobic (Pi-alkyl) | EcoTrx1:TRP31 (Pi-orbitals) | PAPS red:ARG188 (alkyl) | 4.47438 |
| EcoTrx1:TRP31 – PAPS red:ARG188 | Hydrophobic (Pi-alkyl) | EcoTrx1:TRP31 (Pi-orbitals) | PAPS red:ARG188 (alkyl) | 4.03231 |
| EcoTrx1:TRP31 – PAPS red:CYS239 | Hydrophobic (Pi-alkyl) | EcoTrx1:TRP31 (Pi-orbitals) | PAPS red:CYS239 (alkyl) | 5.07597 |

| EcoTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| GLU30 | | + | | | |
| TRP31 | | | | +++++ | |
| PRO34 | | | | ++ | |
| LYS36 | + | + | + | ++ | |
| ILE60 | | | | + | |
| ARG73 | ++ | ++ | ++ | | |
| ILE75 | | + | | + | |
| ALA93 | | + | | | |

## 2. Contact residues of HsTrx1 in its crystal complexes with protein ligands

### 2.1. HsTrx1-SlrP (PDB: 4PUF) [4].

| Interacting residues (SlrP-HsTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| SlrP:TYR424:OH - HsTrx1:GLU88:O | Hydrogen Bond (conventional) | SlrP:TYR424:OH (H-donor) | HsTrx1:GLU88:O (H-Acceptor) | 2.46475 |
| SlrP:SER457:N - HsTrx1:MET74:O | Hydrogen Bond (conventional) | SlrP:SER457:N (H-donor) | HsTrx1:MET74:O (H-Acceptor) | 2.63933 |
| SlrP:VAL459:N - HsTrx1:LYS72:O | Hydrogen Bond (conventional) | SlrP:VAL459:N (H-donor) | HsTrx1:LYS72:O (H-Acceptor) | 3.35557 |
| HsTrx1:ALA92:N - SlrP:ASP455:O | Hydrogen Bond (conventional) | HsTrx1:ALA92:N (H-donor) | SlrP:ASP455:O (H-Acceptor) | 2.63262 |
| HsTrx1:PRO75:CD - SlrP:ASP455:O | Hydrogen Bond (carbon) | HsTrx1:PRO75:CD (H-donor) | SlrP:ASP455:O (H-Acceptor) | 3.69592 |
| HsTrx1:CYS73:SG - SlrP:PHE456 | Other Pi-Sulfur | HsTrx1:CYS73:SG (Sulfur) | SlrP:PHE456 (Pi-orbitals) | 4.44873 |
| SlrP:VAL459 - HsTrx1:VAL59 | Hydrophobic (alkyl) | SlrP:VAL459 (alkyl) | HsTrx1:VAL59 (alkyl) | 4.64785 |
| SlrP:VAL459 - HsTrx1:MET74 | Hydrophobic (alkyl) | SlrP:VAL459 (alkyl) | HsTrx1:MET74 (alkyl) | 4.87158 |
| HsTrx1:LYS96 - SlrP:MET453 | Hydrophobic (alkyl) | HsTrx1:LYS96 (alkyl) | SlrP:MET453 (alkyl) | 4.26638 |

| HsTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| VAL59 | | | | + | |
| LYS72 | | + | | | |
| CYS73 | | | | | + |
| MET74 | | + | | + | |
| PRO75 | | + | | | |
| GLU88 | | + | | | |
| ALA92 | | + | | | |
| LYS96 | | | | + | |

### 2.2. HsTrx1-TrxR (PDB: 3QFA) [5].

| Interacting residues (TrxR-HsTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| TrxR:ARG121:NH1 - HsTrx1:GLU70:OE2 | Hydrogen Bond;Electrostatic (Salt Bridge) | TrxR:ARG121:NH1 (H-donor) | HsTrx1:GLU70:OE2 | 3.74249 |
| TrxR:ARG117:NH1 - HsTrx1:ASP60:OD1 | Electrostatic (attractive charge) | TrxR:ARG117:NH1 (positive) | HsTrx1:ASP60:OD1 | 5.19949 |
| TrxR:ARG121:NH2 - HsTrx1:GLU70:OE1 | Electrostatic (attractive charge) | TrxR:ARG121:NH2 (positive) | HsTrx1:GLU70:OE1 | 5.53065 |
| TrxR:LYS124:NZ - HsTrx1:GLU70:OE1 | Electrostatic (attractive charge) | TrxR:LYS124:NZ (positive) | HsTrx1:GLU70:OE1 | 5.0851 |

| | | | | |
|---|---|---|---|---|
| HsTrx1:LYS36:NZ - TrxR:GLU103:OE2 | Electrostatic (attractive charge) | HsTrx1:LYS36:NZ (positive) | TrxR:GLU103:OE2 | 5.00342 |
| HsTrx1:LYS72:NZ - TrxR:GLU122:OE2 | Electrostatic (attractive charge) | HsTrx1:LYS72:NZ (positive) | TrxR:GLU122:OE2 | 3.91194 |
| TrxR:TRP114:NE1 - HsTrx1:LYS72:O | Hydrogen Bond (conventional) | TrxR:TRP114:NE1 (H-donor) | HsTrx1:LYS72:O (H-acceptor) | 2.72736 |
| TrxR:ARG117:NH2 - HsTrx1:VAL59:O | Hydrogen Bond (conventional) | TrxR:ARG117:NH2 (H-donor) | HsTrx1:VAL59:O (H-acceptor) | 2.76195 |
| TrxR:ARG121:NH2 - HsTrx1:VAL71:O | Hydrogen Bond (conventional) | TrxR:ARG121:NH2 (H-donor) | HsTrx1:VAL71:O (H-acceptor) | 2.91987 |
| HsTrx1:MET74:CE - TrxR:TRP114 | Hydrophobic (Pi-Sigma) | HsTrx1:MET74:CE (C-H) | TrxR:TRP114 (Pi-orbitals) | 3.22536 |
| HsTrx1:MET74:CE - TrxR:TRP114 | Hydrophobic (Pi-Sigma) | HsTrx1:MET74:CE (C-H) | TrxR:TRP114 (Pi-orbitals) | 3.99918 |
| TrxR:GLY110:C.O;SER111:N - HsTrx1:TRP31 | Hydrophobic (amide-Pi stacked) | TrxR:GLY110:C.O;SER111:N (amide) | HsTrx1:TRP31 (Pi-orbitals) | 3.79927 |
| TrxR:GLY110:C.O;SER111:N - HsTrx1:TRP31 | Hydrophobic (amide-Pi stacked) | TrxR:GLY110:C.O;SER111:N (amide) | HsTrx1:TRP31 (Pi-orbitals) | 3.80979 |
| TrxR:VAL118 - HsTrx1:LYS72 | Hydrophobic (alkyl) | TrxR:VAL118 (alkyl) | HsTrx1:LYS72 (alkyl) | 5.01552 |
| TrxR:TRP114 - HsTrx1:VAL59 | Hydrophobic (Pi-alkyl) | TrxR:TRP114 (Pi-orbitals) | HsTrx1:VAL59 (alkyl) | 5.18936 |
| TrxR:TRP114 - HsTrx1:VAL59 | Hydrophobic (Pi-alkyl) | TrxR:TRP114 (Pi-orbitals) | HsTrx1:VAL59 (alkyl) | 4.12479 |
| TrxR:TRP114 - HsTrx1:ALA66 | Hydrophobic (Pi-alkyl) | TrxR:TRP114 (Pi-orbitals) | HsTrx1:ALA66 (alkyl) | 4.70456 |
| TrxR:TRP114 - HsTrx1:VAL71 | Hydrophobic (Pi-alkyl) | TrxR:TRP114 (Pi-orbitals) | HsTrx1:VAL71 (alkyl) | 5.30522 |

| HsTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| TRP31 | | | | ++ | |
| LYS36 | + | | | | |
| VAL59 | | + | | ++ | |
| ASP60 | + | | | | |
| ALA66 | | | | + | |
| GLU70 | ++ | | + | | |
| VAL71 | | + | | + | |
| LYS72 | + | + | | + | |
| MET74 | | | | + | |

### 2.3. HsTrx1-Txnip (PDB: 4LL4) [6]

| Interacting residues (Txnip-HsTrx1) | Category (type) | From (chemistry) | To (chemistry) | Distance (Å) |
|---|---|---|---|---|
| Txnip:ARG251:NH2 - HsTrx1:ASP60:OD2 | Hydrogen Bond;Electrostatic (Salt Bridge) | Txnip:ARG251:NH2 (H-donor) | HsTrx1:ASP60:OD2 (H-acceptor) | 3.00975 |
| Txnip:CYS247:N - | Hydrogen Bond | Txnip:CYS247:N | HsTrx1:MET74:O | 2.92279 |

| | | | | |
|---|---|---|---|---|
| HsTrx1:MET74:O | (conventional) | (H-donor) | (H-acceptor) | |
| HsTrx1:GLY33:N - Txnip:GLU202:OE2 | Hydrogen Bond (conventional) | HsTrx1:GLY33:N (H-donor) | Txnip:GLU202:OE2 (H-acceptor) | 3.14123 |
| HsTrx1:MET74:N - Txnip:CYS247:O | Hydrogen Bond (conventional) | HsTrx1:MET74:N (H-donor) | Txnip:CYS247:O (H-acceptor) | 2.85886 |
| HsTrx1:ALA92:N - Txnip:GLY245:O | Hydrogen Bond (conventional) | HsTrx1:ALA92:N (H-donor) | Txnip:GLY245:O (H-acceptor) | 3.17731 |
| Txnip:ASP200:OD1 - HsTrx1:TRP31 | Electrostatic (Pi-anion) | Txnip:ASP200:OD1 (negative) | HsTrx1:TRP31 (Pi-orbitals) | 3.94097 |
| Txnip:ASP200:OD2 - HsTrx1:TRP31 | Electrostatic (Pi-anion) | Txnip:ASP200:OD2 (negative) | HsTrx1:TRP31 (Pi-orbitals) | 3.87899 |
| Txnip:CYS247 - HsTrx1:CYS32 | Hydrophobic (alkyl) | Txnip:CYS247 (alkyl) | HsTrx1:CYS32 (alkyl) | 3.30414 |
| Txnip:CYS247 - HsTrx1:PRO34 | Hydrophobic (alkyl) | Txnip:CYS247 (alkyl) | HsTrx1:PRO34 (alkyl) | 4.98945 |
| Txnip:CYS247 - HsTrx1:MET74 | Hydrophobic (alkyl) | Txnip:CYS247 (alkyl) | HsTrx1:MET74 (alkyl) | 5.44584 |
| Txnip:ALA248 - HsTrx1:CYS73 | Hydrophobic (alkyl) | Txnip:ALA248 (alkyl) | HsTrx1:CYS73 (alkyl) | 5.00429 |
| HsTrx1:TRP31 - Txnip:CYS247 | Hydrophobic (Pi-alkyl) | HsTrx1:TRP31 (Pi-orbitals) | Txnip:CYS247 (alkyl) | 4.7896 |

| HsTrx1 interacting residues | Electrostatic interaction | Hydrogen bonding | Salt bridge | Hydrophobic interaction | Other |
|---|---|---|---|---|---|
| TRP31 | ++ | | | + | |
| CYS32 | | | | + | |
| GLY33 | | + | | | |
| PRO34 | | | | + | |
| ASP60 | + | + | | | |
| CYS73 | | | | + | |
| MET74 | | ++ | | + | |
| AΛA92 | | + | | | |

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