**S5 Table. Internal SOD1 disulphide sub-loop hydrogen bonding in the disulphide intact homodimeric state in comparison with the conformation present in heterodimeric complex with hCCS.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Amino Acid** | **Group (atom)** | **Distance** | **Group (atom)** | **Amino Acid** |
|  |  | SOD1 homodimer | SOD1complex |  |  |
| **Conserved** |  |  |  |  |  |
| His48 | Imidazole (ND1) | 2.82 Å | 2.88 Å | Carbonyl (O) | Gly61 |
| Glu49 | Amine (N) | 2.90 Å | 2.85 Å | Carbonyl (O) | Pro62 |
| Phe50 | Amine (N) | 3.02 Å | 3.03 Å | Carbonyl (O) | Ala60 |
| Thr54 | Amine (N) | 2.89 Å | 3.34 Å | Carboxylate (OD1) | Asp52 |
| Thr54 | Side-chain OH (OG1) | 2.66 Å | 2.60 Å | Carboxylate (OD1) | Asp52 |
| Ala55 | Amine (N) | 2.81 Å | 2.60 Å | Side-chain OH (OG) | Ser59 |
| Ser59 | Side-chain OH (OG) | 3.42 Å | 2.95 Å | Carbonyl (O) | Gly56 |
|  |  |  |  |  |  |
| **Rearranged** |  |  |  |  |  |
| Ala60 | Amine (N) | 3.16 Å | N/A | Carbonyl (O) | Cys57 |
| Ala60 | Amine (N) | N/A | 3.24 Å | Carbonyl (O) | Gly56 |
|  |  |  |  |  |  |
| Gly61 | Amine (N) | 3.23 Å | N/A | Carbonyl (O) | Th58 |
| Gly61 | Amine (N) | N/A | 3.06 Å | Carbonyl (O) | Ala57\* |
|  |  |  |  |  |  |
| **Lost** |  |  |  |  |  |
| Gly56 | Amine (N) | 3.03 Å | N/A | Carbonyl (O) | Asn53 |
| Ser59 | Amine (N) | 3.14 Å | N/A | Carbonyl (O) | Gly56 |
|  |  |  |  |  |  |
| **Gained** |  |  |  |  |  |
| Thr58 | Amine (N) | N/A | 3.30 Å | Carbonyl (O) | Ala55 |
| Ser59 | Side-chain OH (OG) | N/A | 3.05 Å | Carbonyl (O) | Asp52 |

\*Ala57 substituted for Cys57.