**Supplementary File 7:** List of interactions# involving the catalytic triad residues S137, D258 and H286.

|  |  |  |
| --- | --- | --- |
| **Source atoms**  | **Target atoms**  | **Distance (Å)** |
| *Monomer A*Ser 137A NSer 137A Oconformation ASer 137 A OGconformation BSer 137 A OGAsp 258A NAsp 258A OD1Asp 258A OD2His 286A NHis 286A ND1His 286A NE2His 286A O*Monomer B*Ser 137B NSer 137B Oconformation ASer 137B OG conformation BSer 137B OGAsp 258B NAsp 258B OD1Asp 258B OD2His 286B NHis 286B ND1His 286B NE2His 286B O | Asn 136A ND2Ile 160A OAsp 161A OAla 163A NGly 139A NGly 140A NHis 141A NHis 286A NE2HOH 229S OMYR 500A O1HOH 229S OGly 255A OLeu 261A OLeu 261A NHis 286A ND1Arg 259A NVal 260A NTrp 254A NE1Leu 261A OAsp 161A OD2His 286A ND1Val 199A OAsp 258A OD1Asp 258A OD2Ser 137A OGAsn 136A ND2Asn 136B ND2Ile 160B OAsp 161B OAla 163B NGly 140B NHis 141B NGly 139B NHis 286B NE2HOH 171S OIPA 504B C1<<<HOH 171S OGly 255B OArg 259B NLeu 261B NLeu 261B OVal 260B NHis 286B ND1Trp 254B NE1Asp 161B OD2Leu 261B OHis 286B ND1Val 199B OAsp 258B OD2Asp 258B OD1Ser 137B OGAsn 136B ND2 | 3.393.203.043.013.172.892.973.042.233.432.523.133.252.933.123.002.753.493.082.632.723.083.122.723.043.253.353.163.053.022.893.023.192.832.623.252.803.082.972.943.292.773.123.432.673.222.722.972.723.122.833.16 |

#The cut-off value for hydrogen bond selection used is ≤ 3.5 Å.