|  |  |  |  |
| --- | --- | --- | --- |
| Complex  (Protein-ligand) | ΔGbind  (kcal/mol) | Amino acids that interact through hydrogen bonds (distance) | Amino acids that make hydrophobic interactions |
| 4did\_gdp (controle) | -6.1 | 3.05 (leu 160 N – gdp 200 06)  3.10 (gly 15 N – gdp 200 O3B)  3.15 (ala 159 N – gdp 200 O6)  3.21 (cys 18 N – gdp 200 O2B) | Thr17  Ala13  Val33  Phe28  Ser158  Asp118  Gln116 |
| 4did\_0q4 | -5.5 | 2.81 (thr 125 OG1 - 0q4 125 N7)  2.98 (gln 116 OE1 - 0q4 NH1)  3.09 (ala 13 O - 0q4 NH1)  3.11 (leu 160 N - 0q4 125 OE1)  3.17 (gln 116 OE1 - 0q4 125 NH2)  3.22 (ser 124 OG - 0q4 125 N7) | Val33  Cys18  Ser30  Phe28  Leu119  Ala159  Lys128  Val85  Leu129 |
| 4did\_31g | -6.6 | 2.83 (asp 118 OD1 - 31g 401 N3)  3.09 (cys 18 N - 31g 401 O1)  3.09 (ser 158 OG - 31g 401 N3)  3.16 (asp 118 OD1 - 31g 401 N2)  3.34 (gly 15 N - 31g 401 O2) | Thr17  Ala13  Val33  Phe28  Gln116  Leu160 |
| 4did\_nag | -5.4 | 2.96 (leu 160 N – nag 700 O4)  2.98 (gln 116 N – nag 700 O6)  3.00 (ala 159 N – nag 700 O6)  3.05 (ala 159 N – nag 700 O4)  3.07 (gln 116 NE2 – nag 700 O5)  3.11 (asp 118 OD1 – nag 700 O4)  3.15 (ser 158 OG – nag 700 O4) | Phe28  Leu119 |