**Supplementary Data:**

**Supplementary -Table 1:**

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| **Protein** | **Ligand** | **Interacting Amino Acids** | **Energy (kcal/mol)** |
| **ATP** | **dATP** | **ATP** | **dATP** |
| **Wild Type** | Ligand 1 | GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206TYR 277 | GLU 80SER 81GLY 83THR 85THR 86ALA 110 | -8.0 | -7.5 |
| Ligand 2 | SER 81GLY 83LYS 84THR 85THR 86TYR 115ASP 156VAL 251LEU 275TYR 277LYS 239 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206LEU 275TYR 277 | -7.5 | -7.3 |
| Ligand 3 | SER 81GLY 83LYS 84THR 85THR 86GLU 108ALA 110GLN 206LYS 239 | GLU 80SER 81GLY 83LYS 84THR 85THR 86GLN 206LYS 239TYR 277 | -7.2 | -7.2 |
| Ligand 4 | GLU 80LYS 84THR 85LYS 239LEU 276TYR 277 | GLU 80GLY 83LYS 84THR 85GLU 108ASP 112TYR 115GLN 206LEU 275 | -7.1 | -6.5 |
| Ligand 5 | GLU 80SER 81GLY 83LYS 84THR 85ASP 112TYR 115GLN 206 | GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115 | -6.9 | -6.4 |
| Ligand 6 | GLY 83LYS 84THR 85THR 86TYR 115GLN 206TYR 277 | GLU 80SER 81THR 85GLU 108ALA 110ASP 112TYR 115ASP 156GLN 206LYS 239 | -6.9 | -6.4 |
| Ligand 7 | SER 81GLY 83LYS 84THR 85THR 86TYR 115LYS 239VAL 251LEU 275TYR 277 | SER 81LYS 84THR 85ASP 112TYR 115GLN 206LEU 275 | -6.9 | -6.3 |
| Ligand 8 | GLU 80THR 86GLU 108ASP 156GLN 206 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 156LEU 275 | -6.8 | -6.3 |
| Ligand 9 | SER 81LYS 84THR 85THR 86GLU 108ASP 156GLN 206 | SER 81THR 85THR 86ALA 110ASP 112LYS 239LEU 275TYR 277 | -6.8 | -6.3 |

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| **Protein** | **Ligand** | **Interacting Amino Acids** | **Energy (kcal/mol)** |
| **ATP** | **dATP** | **ATP** | **dATP** |
| **77p** | Ligand 1 | GLU 80GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206LEU 275TYR 277 | GLU 80SER 81GLY 83THR 85THR 86ALA 110TYR 277 | -7.7 | -7.5 |
| Ligand 2 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 156GLN 206LYS 239LEU 275TYR 277 | GLU 80SER 81GLY 83LYS 84THR85THR 86GLN 206LYS 239TYR 277 | -7.6 | -7.0 |
| Ligand 3 | SER 81GLY 83LYS 84THR 85THR 86TYR 115LYS 239VAL 251TYR 277 | GLY 83LYS 84THR 85THR 86ALA 110 | -7.4 | -6.7 |
| Ligand 4 | GLU 80SER 81GLY 83THR 85THR 86ALA 110ASP 112TYR 115TYR 277 | GLU 80SER 81GLY 83LYS 84THR 85ASP 112TYR 115ASP 156GLN 206LEU 275TYR 277 | -7.4 | -6.5 |
| Ligand 5 | GLU 80SER 81LYS 84THR 85THR 86GLN 206LYS 239LEU 275TYR 277 | SER 81GLY 83LYS 84THR 85THR 86LYS 239VAL 251TYR 277 | -7.2 | -6.5 |
| Ligand 6 | SER 81GLY 83LYS 84THR 85THR 86GLU 108ASP 156GLN 206LEU 275 | THR 85THR 86ALA 110ASP 112TYR 115LEU 275TYR 277 | -7.2 | -6.5 |
| Ligand 7 | GLU 80SER 81GLY 83LYS 84THR 85THR 86GLU 108ALA 110ASP 156GLN 206 | GLU 80SER 81LYS 84THR 85THR 86ASP 112TYR 115GLN 206LEU 275 | -7.2 | -6.5 |
| Ligand 8 | SER 81LYS 84THR 85THR 86GLU 108ASP 156GLN 206LYS 239 | SER 81THR 86LYS 239LEU 275TYR 277 | -7.2 | -6.4 |
| Ligand 9 | GLU 80SER 81GLY 83LYS 84THR 85TYR 115GLN 206 | SER 81GLY 83LYS 84THR 85ASP 112TYR 115ASP 156LEU 275 | -7.2 | -6.4 |

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| --- | --- | --- | --- |
| **Protein** | **Ligand** | **Interacting Amino Acids** | **Energy (kcal/mol)** |
| **ATP** | **dATP** | **ATP** | **dATP** |
| **318P** | Ligand 1 | GLU 80SER 81GLY 83LYS 84THR 85THR 86GLN 206LYS 239VAL 251LEU 275TYR 277 | GLU 80SER 81GLY 83THR 85THR 86ALA 110TYR 277 | -8.5 | -7.4 |
| Ligand 2 | GLU 80SER 81GLY 83THR 85THR 86ALA 110ASP 112TYR 115LYS 239TYR 277 | GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115ASP 156GLN 206TYR 277 | -8.4 | -7.0 |
| Ligand 3 | GLU 80SER 81GLY 83LYS 84THR 85THR 86LYS 239VAL 251LEU 275TYR 277 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 156GLN 206LYS 239TYR 277 | -8.0 | -6.9 |
| Ligand 4 | GLU 80SER 81LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206TYR 277 | SER 81GLY 83LYS 84THR 85THR 86LYS 239TYR 277 | -8.0 | -6.6 |
| Ligand 5 | SER 81GLY 83LYS 84THR 85THR 86ALA 110GLN 206 | SER 81LYS 84THR 85THR 86ASP 112TYR 115LEU 275TYR 277 | -7.9 | -6.5 |
| Ligand 6 | GLU 80SER 81LYS 84THR 85THR 86GLN 206LYS 239LEU 275TYR 277 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 112TYR 115GLN 206LEU 275 | -7.7 | -6.5 |
| Ligand 7 | GLY 83LYS 84THR 85THR 86ASP 112TYR 115 | GLU 80GLY 83LYS 84THR 85THR 86ASP 112TYR 115GLN 206LEU 275TYR 277 | -7.7 | -6.4 |
| Ligand 8 | GLU 80GLY 83LYS 84THR 85THR 86GLU 108TYR 115GLN 206 | GLU 80SER 81THR 85ALA 110ASP 112TYR 115LYS 239LEU 275 | -7.7 | -6.2 |
| Ligand 9 | GLU 80GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115TYR 277 | SER 81GLY 83THR 85THR 86GLU 108GLN 206ASP 156 | -7.6 | -6.2 |

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| --- | --- | --- | --- |
| **Protein** | **Ligand** | **Interacting Amino Acids** | **Energy (kcal/mol)** |
| **ATP** | **dATP** | **ATP** | **dATP** |
| **77p 318p** | Ligand 1 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ALA 110TYR 115LYS 239TYR 277 | GLU 80GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206TYR 277 | -7.5 | -8.0 |
| Ligand 2 | SER 81GLY 83LYS 84THR 85THR 86GLU 108ALA 110ASP 156GLN 206 | GLU 80SER 81GLY 83THR 85THR 86ALA 110ASP 112 | -7.0 | -8.0 |
| Ligand 3 | GLU 80GLY 83LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206TYR 277 | GLU 80SER 81GLY 83LYS 84THR 85THR 86TYR 115ASP 156GLN 206LYS 239TYR 277 | -7.0 | -7.5 |
| Ligand 4 | GLU 80SER 81LYS 84THR 85THR 86GLU 108TYR 115ASP 156GLN 206LYS 239LEU 275TYR 277 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 112TYR 115LEU 275TYR 277 | -6.6 | -7.3 |
| Ligand 5 | GLU 80LYS 84THR 85THR 86GLU 108ASP 112TYR 115GLN 206LEU 275TYR 277 | GLU 80LYS 84THR 86ASP 112TYR 115GLN 206TYR 277 | -6.6 | -7.2 |
| Ligand 6 | GLU 80SER 81GLY 83LYS 84THR 85THR 86LYS 239LEU 275TYR 277 | SER 81GLY 83LYS 84THR 85ALA 110ASP 112TYR 115ASP 156LEU 275 | -6.6 | -6.9 |
| Ligand 7 | GLU 80SER 81GLY 83LYS 84THR 85THR 86ASP 112TYR 115LEU 275 | GLU 80SER 81LYS 84THR 85THR 86GLU 108ASP 156GLN 206 | -6.4 | -6.9 |
| Ligand 8 | GLU 80SER 81LYS 84THR 85THR 86ALA 110TYR 115GLN 206LYS 239LEU 275TYR 277 | GLU 80SER 81LYS 84THR 85THR 86ALA 110ASP 112TYR 115GLN 206LEU 275TYR 277 | -6.4 | -6.8 |
| Ligand 9 | SER 81THR 85THR 86ALA 110LEU 111ASP 112LEU 275 | SER 81GLY 83THR 85THR 86TYR 115TYR 277 | -6.4 | -6.8 |

**Supplementary Figure 1;** Aligned docked poses of **(A)** DrRecA (green) with T318p (cyan), and **(B)** DrRecA (green) with Y77pT318p (magenta)

