**Supplementary Data:**

**Supplementary -Table 1:**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Protein** | **Ligand** | **Interacting Amino Acids** | | **Energy (kcal/mol)** | |
| **ATP** | **dATP** | **ATP** | **dATP** |
| **Wild Type** | Ligand 1 | GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  TYR 277 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110 | -8.0 | -7.5 |
| Ligand 2 | SER 81  GLY 83  LYS 84  THR 85  THR 86  TYR 115  ASP 156  VAL 251  LEU 275  TYR 277  LYS 239 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  LEU 275  TYR 277 | -7.5 | -7.3 |
| Ligand 3 | SER 81  GLY 83  LYS 84  THR 85  THR 86  GLU 108  ALA 110  GLN 206  LYS 239 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  GLN 206  LYS 239  TYR 277 | -7.2 | -7.2 |
| Ligand 4 | GLU 80  LYS 84  THR 85  LYS 239  LEU 276  TYR 277 | GLU 80  GLY 83  LYS 84  THR 85  GLU 108  ASP 112  TYR 115  GLN 206  LEU 275 | -7.1 | -6.5 |
| Ligand 5 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  ASP 112  TYR 115  GLN 206 | GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115 | -6.9 | -6.4 |
| Ligand 6 | GLY 83  LYS 84  THR 85  THR 86  TYR 115  GLN 206  TYR 277 | GLU 80  SER 81  THR 85  GLU 108  ALA 110  ASP 112  TYR 115  ASP 156  GLN 206  LYS 239 | -6.9 | -6.4 |
| Ligand 7 | SER 81  GLY 83  LYS 84  THR 85  THR 86  TYR 115  LYS 239  VAL 251  LEU 275  TYR 277 | SER 81  LYS 84  THR 85  ASP 112  TYR 115  GLN 206  LEU 275 | -6.9 | -6.3 |
| Ligand 8 | GLU 80  THR 86  GLU 108  ASP 156  GLN 206 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 156  LEU 275 | -6.8 | -6.3 |
| Ligand 9 | SER 81  LYS 84  THR 85  THR 86  GLU 108  ASP 156  GLN 206 | SER 81  THR 85  THR 86  ALA 110  ASP 112  LYS 239  LEU 275  TYR 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 80  GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110  TYR 277 | -7.7 | -7.5 |
| Ligand 2 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 156  GLN 206  LYS 239  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR85  THR 86  GLN 206  LYS 239  TYR 277 | -7.6 | -7.0 |
| Ligand 3 | SER 81  GLY 83  LYS 84  THR 85  THR 86  TYR 115  LYS 239  VAL 251  TYR 277 | GLY 83  LYS 84  THR 85  THR 86  ALA 110 | -7.4 | -6.7 |
| Ligand 4 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110  ASP 112  TYR 115  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  ASP 112  TYR 115  ASP 156  GLN 206  LEU 275  TYR 277 | -7.4 | -6.5 |
| Ligand 5 | GLU 80  SER 81  LYS 84  THR 85  THR 86  GLN 206  LYS 239  LEU 275  TYR 277 | SER 81  GLY 83  LYS 84  THR 85  THR 86  LYS 239  VAL 251  TYR 277 | -7.2 | -6.5 |
| Ligand 6 | SER 81  GLY 83  LYS 84  THR 85  THR 86  GLU 108  ASP 156  GLN 206  LEU 275 | THR 85  THR 86  ALA 110  ASP 112  TYR 115  LEU 275  TYR 277 | -7.2 | -6.5 |
| Ligand 7 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  GLU 108  ALA 110  ASP 156  GLN 206 | GLU 80  SER 81  LYS 84  THR 85  THR 86  ASP 112  TYR 115  GLN 206  LEU 275 | -7.2 | -6.5 |
| Ligand 8 | SER 81  LYS 84  THR 85  THR 86  GLU 108  ASP 156  GLN 206  LYS 239 | SER 81  THR 86  LYS 239  LEU 275  TYR 277 | -7.2 | -6.4 |
| Ligand 9 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  TYR 115  GLN 206 | SER 81  GLY 83  LYS 84  THR 85  ASP 112  TYR 115  ASP 156  LEU 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 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  GLN 206  LYS 239  VAL 251  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110  TYR 277 | -8.5 | -7.4 |
| Ligand 2 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110  ASP 112  TYR 115  LYS 239  TYR 277 | GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  ASP 156  GLN 206  TYR 277 | -8.4 | -7.0 |
| Ligand 3 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  LYS 239  VAL 251  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 156  GLN 206  LYS 239  TYR 277 | -8.0 | -6.9 |
| Ligand 4 | GLU 80  SER 81  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  TYR 277 | SER 81  GLY 83  LYS 84  THR 85  THR 86  LYS 239  TYR 277 | -8.0 | -6.6 |
| Ligand 5 | SER 81  GLY 83  LYS 84  THR 85  THR 86  ALA 110  GLN 206 | SER 81  LYS 84  THR 85  THR 86  ASP 112  TYR 115  LEU 275  TYR 277 | -7.9 | -6.5 |
| Ligand 6 | GLU 80  SER 81  LYS 84  THR 85  THR 86  GLN 206  LYS 239  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 112  TYR 115  GLN 206  LEU 275 | -7.7 | -6.5 |
| Ligand 7 | GLY 83  LYS 84  THR 85  THR 86  ASP 112  TYR 115 | GLU 80  GLY 83  LYS 84  THR 85  THR 86  ASP 112  TYR 115  GLN 206  LEU 275  TYR 277 | -7.7 | -6.4 |
| Ligand 8 | GLU 80  GLY 83  LYS 84  THR 85  THR 86  GLU 108  TYR 115  GLN 206 | GLU 80  SER 81  THR 85  ALA 110  ASP 112  TYR 115  LYS 239  LEU 275 | -7.7 | -6.2 |
| Ligand 9 | GLU 80  GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  TYR 277 | SER 81  GLY 83  THR 85  THR 86  GLU 108  GLN 206  ASP 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 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ALA 110  TYR 115  LYS 239  TYR 277 | GLU 80  GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  TYR 277 | -7.5 | -8.0 |
| Ligand 2 | SER 81  GLY 83  LYS 84  THR 85  THR 86  GLU 108  ALA 110  ASP 156  GLN 206 | GLU 80  SER 81  GLY 83  THR 85  THR 86  ALA 110  ASP 112 | -7.0 | -8.0 |
| Ligand 3 | GLU 80  GLY 83  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  TYR 115  ASP 156  GLN 206  LYS 239  TYR 277 | -7.0 | -7.5 |
| Ligand 4 | GLU 80  SER 81  LYS 84  THR 85  THR 86  GLU 108  TYR 115  ASP 156  GLN 206  LYS 239  LEU 275  TYR 277 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 112  TYR 115  LEU 275  TYR 277 | -6.6 | -7.3 |
| Ligand 5 | GLU 80  LYS 84  THR 85  THR 86  GLU 108  ASP 112  TYR 115  GLN 206  LEU 275  TYR 277 | GLU 80  LYS 84  THR 86  ASP 112  TYR 115  GLN 206  TYR 277 | -6.6 | -7.2 |
| Ligand 6 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  LYS 239  LEU 275  TYR 277 | SER 81  GLY 83  LYS 84  THR 85  ALA 110  ASP 112  TYR 115  ASP 156  LEU 275 | -6.6 | -6.9 |
| Ligand 7 | GLU 80  SER 81  GLY 83  LYS 84  THR 85  THR 86  ASP 112  TYR 115  LEU 275 | GLU 80  SER 81  LYS 84  THR 85  THR 86  GLU 108  ASP 156  GLN 206 | -6.4 | -6.9 |
| Ligand 8 | GLU 80  SER 81  LYS 84  THR 85  THR 86  ALA 110  TYR 115  GLN 206  LYS 239  LEU 275  TYR 277 | GLU 80  SER 81  LYS 84  THR 85  THR 86  ALA 110  ASP 112  TYR 115  GLN 206  LEU 275  TYR 277 | -6.4 | -6.8 |
| Ligand 9 | SER 81  THR 85  THR 86  ALA 110  LEU 111  ASP 112  LEU 275 | SER 81  GLY 83  THR 85  THR 86  TYR 115  TYR 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)

