Files used per sample:

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **pdb Files** | | | | | | | | | |
| WT | 207 | 216 | 589 | 814 | 1384 | 1478 | 1579 | 1808 | 1914 | 2296 |
| K75G | 22 | 55 | 90 | 125 | 235 | 325 | 420 | 575 | 1155 | 2070 |
| R78G | 1032 | 1035 | 1414 | 1415 | 1430 | 1436 | 1439 | 1461 | 1463 | 1469 |
| K75G-R78G | 59 | 996 | 1277 | 1584 | 1949 | 2103 | 2223 | 2225 | 2228 | 2404 |

Single water bridges:

|  |  |  |  |
| --- | --- | --- | --- |
| **WT** | **K75G** | **R78G** | **K75G-R78G** |
| A0007-B0001  A0007-B0006  A0013-B0002 | A0006-B0035  A0019-B0031  A0024-B0034  A0024-B0035 | A0008-B0032  A0011-B0029  A0024-B0035  A0024-B0038  A0026-B0038 | A0001-B0029  A0002-B0029  A0004-B0029  A0007-B0036  A0008-B0033  A0013-B0041  A0022-B0031  A0025-B0031  A0026-B0030 |

Double water bridges:

|  |  |  |  |
| --- | --- | --- | --- |
| **WT** | **K75G** | **R78G** | **K75G-R78G** |
| A0007-B0001  A0007-B0003 | A0008-B0030  A0019-B0029  A0019-B0031 | A0004-B0035  A0008-B0032  A0010-B0030  A0010-B0031  A0011-B0030  A0021-B0031  A0024-B0038  A0025-B0036  A0025-B0038  A0026-B0042 | A0005-B0036  A0007-B0042  A0008-B0033  A0020-B0029  A0020-B0033  A0021-B0033 |