**Supporting Information**

**Effect of sequence and stereochemistry reversal on p53 peptide mimicry**

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**Figure S1.** Replica exchange equilibration for the (initially) 270 K replica.



**Figure S2.** 310 helical content from REMD simulations of **WT**, **I**, **R** and **RI**.



**Table S1** Averagenumber of hydrogen bonds between the backbone peptide C=O of residues *i* and the backbone peptide NH of the residues *i + 4* and average total number of hydrogen bonds within sequence over final 20 ns of REMD for sequences **WT**, **I**, **R** and **RI**. Standard deviations in parentheses.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| ***i → i+4*** | ***i(WT/I)*** | ***i(R/RI)*** | **WT** | **I** | **R** | **RI** |
| 0 – 4 | Ace | Ace | 0.04 (0.19) | 0.04 (0.19) | 0.00 (0.02) | 0.00 (0.03) |
| 1 – 5 | Ser | Asn | 0.04 (0.21) | 0.04 (0.20) | 0.09 (0.28) | 0.05 (0.22) |
| 2 – 6 | Gln | Glu | 0.11 (0.31) | 0.10 (0.30) | 0.31 (0.46) | 0.30 (0.46) |
| 3 – 7 | Glu | Pro | 0.08 (0.26) | 0.07 (0.25) | 0.18 (0.39) | 0.17 (0.38) |
| 4 – 8 | Thr | Leu | 0.14 (0.34) | 0.12 (0.33) | 0.26 (0.44) | 0.23 (0.42) |
| 5 – 9 | Phe | Leu | 0.16 (0.37) | 0.18 (0.39) | 0.28 (0.45) | 0.28 (0.45) |
| 6 – 10 | Ser | Lys | 0.05 (0.22) | 0.06 (0.23) | 0.12 (0.33) | 0.11 (0.32) |
| 7 – 11 | Asp | Trp | 0.05 (0.21) | 0.04 (0.20) | 0.16 (0.37) | 0.14 (0.35) |
| 8 – 12 | Leu | Leu | 0.25 (0.43) | 0.26 (0.44) | 0.15 (0.36) | 0.14 (0.35) |
| 9 – 13 | Trp | Asp | **-** | **-** | 0.05 (0.22) | 0.06 (0.23) |
| 10 – 14 | Lys | Ser | 0.00 (0.00) | 0.00 (0.01) | 0.09 (0.29) | 0.11 (0.31) |
| 11 – 15 | Leu | Phe | 0.02 (0.15) | 0.01 (0.12) | 0.15 (0.36) | 0.14 (0.35) |
| *total* |  |   | 0.94 (0.92) | 0.93 (0.91) | 1.84 (1.48) | 1.74 (1.45) |