**SUPPORTING INFORMATION**

# Insights into the Molecular Flexibility of Theta-defensins by NMR Relaxation Analysis.

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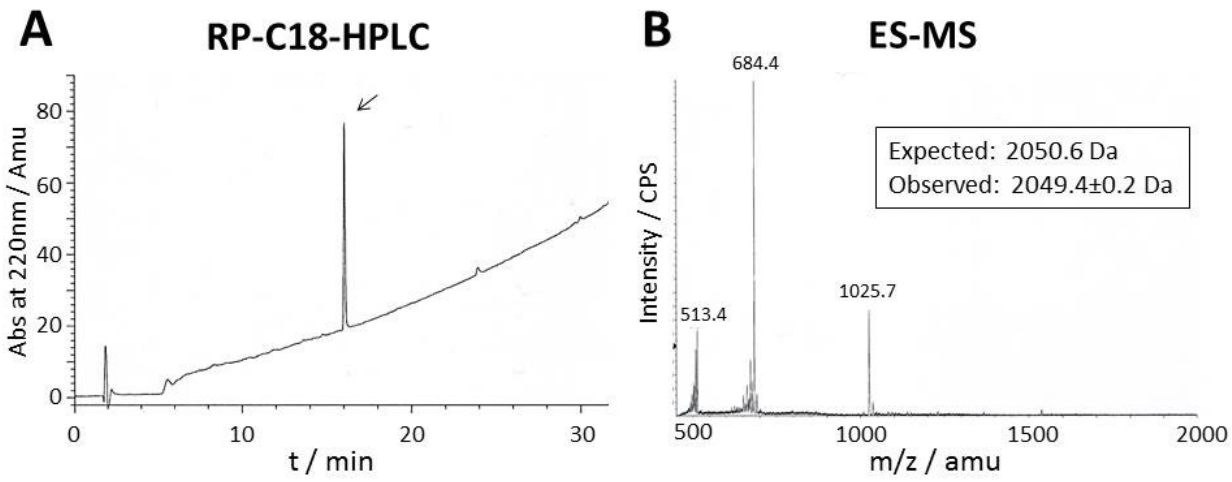
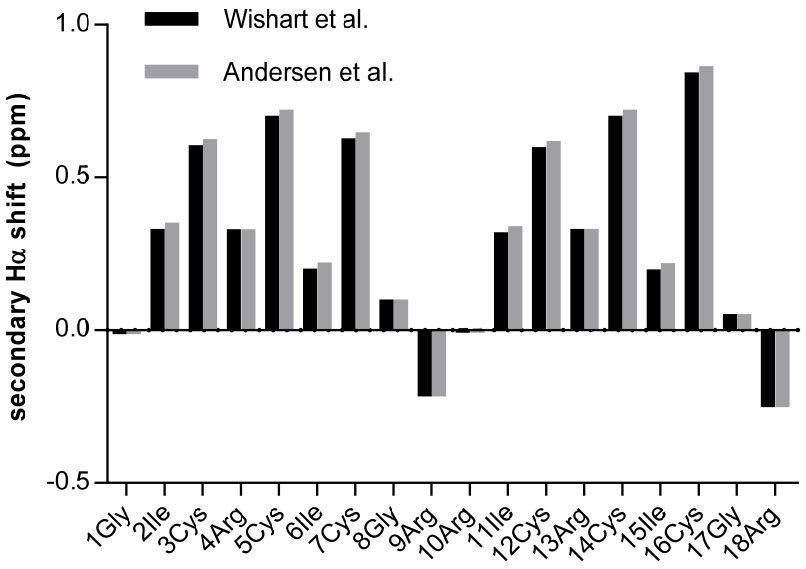



**Figure S1.**Characterization of $^{15}$N-labeled HTD-2. Reverse-phase HPLC analysis (A) and ES-MS analysis (B) of purified $^{15}$N-labeled HTD-2.

**Supplementary Figure S2:** Secondary Hα chemical shifts of HTD-2



**Supplementary Table S1.** Forward (p5) and reverse (p3) 5'-phosphorylated oligonucleotides used to clone the different TEV-HTD2-intein linear precursors into the pTXB1 expression plasmid.

| Peptide | | Oligonucleotide Sequence |
|---|---|---|
| HTD-2 | p5 | 5'-TATGGAAAACCTGTACTTCCAGTGCATCTGCGGTCGTCGTATC TGCCGTTGCATCTGCGGTCGTGGTATCTGCCGT-3' |
| | p3 | 5'-GCAACGGCAGATACCACGACCGCAGATGCAACGGCAGATACG ACGACCGCAGATGCACTGGAAGTACAGGTTTTCCA-3' |

**Supplementary Table S2: T1 relaxation times of $^{15}$N-labelled HTD-2.**

| | 500 MHz | | 600 MHz | | 900 MHz | |
|---|---|---|---|---|---|---|
| **Residue** | **mean** | **s.d.** | **mean** | **s.d.** | **mean** | **s.d.** |
| 1 Gly | 0.57 | 0.04 | 0.65 | 0.02 | 0.71 | 0.05 |
| 2 Ile | 0.57 | 0.02 | 0.60 | 0.01 | 0.61 | 0.01 |
| 3 Cys | | | | | | |
| 4 Arg | 0.59 | 0.02 | 0.58 | 0.02 | 0.57 | 0.01 |
| 5 Cys | 0.56 | 0.01 | 0.60 | 0.01 | 0.63 | 0.01 |
| 6 Ile | 0.54 | 0.01 | 0.56 | 0.03 | 0.56 | 0.00 |
| 7 Cys | 0.53 | 0.01 | 0.57 | 0.01 | 0.57 | 0.00 |
| 8 Gly | 0.55 | 0.01 | 0.57 | 0.01 | 0.63 | 0.00 |
| 9 Arg | 0.61 | 0.01 | 0.65 | 0.01 | 0.64 | 0.01 |
| 10 Arg | 0.67 | 0.04 | 0.69 | 0.02 | | |
| 11 Ile | 0.62 | 0.02 | 0.64 | 0.01 | 0.64 | 0.02 |
| 12 Cys | | | | | | |
| 13 Arg | 0.58 | 0.01 | 0.57 | 0.01 | 0.60 | 0.00 |
| 14 Cys | 0.56 | 0.03 | 0.59 | 0.01 | 0.59 | 0.01 |
| 15 Ile | 0.54 | 0.01 | 0.55 | 0.01 | 0.58 | 0.01 |
| 16 Cys | 0.52 | 0.01 | 0.58 | 0.02 | 0.59 | 0.02 |
| 17 Gly | 0.61 | 0.03 | 0.58 | 0.01 | 0.61 | 0.01 |
| 18 Arg | 0.60 | 0.02 | 0.68 | 0.04 | 0.71 | 0.06 |

**Supplementary Table S3: NOE values of $^{15}$N-labelled HTD-2.**

| | 500 MHz | | 600 MHz | | 900 MHz | |
|---|---|---|---|---|---|---|
| **Residue** | **mean** | **s.d.** | **mean** | **s.d.** | **mean** | **s.d.** |
| 1 Gly | -0.26 | 0.09 | 0.03 | 0.00 | 0.57 | 0.03 |
| 2 Ile | -0.36 | 0.03 | 0.05 | 0.00 | 0.60 | 0.01 |
| 3 Cys | -0.23 | 0.10 | 0.07 | 0.01 | 0.58 | 0.08 |
| 4 Arg | -0.47 | 0.08 | 0.04 | 0.00 | 0.63 | 0.02 |
| 5 Cys | -0.39 | 0.06 | 0.06 | 0.00 | 0.67 | 0.03 |
| 6 Ile | -0.38 | 0.05 | 0.13 | 0.01 | 0.65 | 0.02 |
| 7 Cys | -0.35 | 0.03 | 0.12 | 0.00 | 0.61 | 0.01 |
| 8 Gly | -0.30 | 0.07 | 0.09 | 0.01 | 0.62 | 0.01 |
| 9 Arg | -0.31 | 0.03 | 0.08 | 0.00 | 0.56 | 0.00 |
| 10 Arg | -0.29 | 0.12 | -0.04 | 0.01 | 0.47 | 0.01 |
| 11 Ile | -0.28 | 0.10 | -0.07 | 0.01 | 0.56 | 0.01 |
| 12 Cys | -0.21 | 0.05 | 0.09 | 0.03 | 0.51 | 0.04 |
| 13 Arg | -0.38 | 0.05 | 0.04 | 0.01 | 0.59 | 0.03 |
| 14 Cys | -0.39 | 0.06 | 0.06 | 0.01 | 0.65 | 0.03 |
| 15 Ile | -0.38 | 0.05 | 0.13 | 0.01 | 0.64 | 0.02 |
| 16 Cys | -0.25 | 0.06 | 0.08 | 0.00 | 0.62 | 0.02 |
| 17 Gly | -0.32 | 0.00 | 0.08 | 0.00 | 0.65 | 0.01 |
| 18 Arg | -0.25 | 0.04 | 0.04 | 0.00 | 0.44 | 0.02 |

**Supplementary Table S4.** Experimental NMR relaxation data for HTD-2 and fitted data using ModelFree.

| Residue | Data[a] | $T_1$ (s) | | | NOE | | | θ (°) | $\tau_i$ (ps) | $S^2$ | RMSD[b] |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 500 | 600 | 900 | 500 | 600 | 900 | | | | |
| 1 Gly | *Exp* | *0.57* | *0.65* | *0.71* | *-0.26* | *0.03* | *0.57* | *111* | | | |
| | IsoRigid[c] | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.33 |
| | Ax Rigid[d] | 0.46 | 0.47 | 0.45 | -0.32 | 0.04 | 0.56 | 111 | | | 0.33 |
| | Iso + Int[e] | 0.64 | 0.65 | 0.64 | -0.30 | 0.03 | 0.51 | | 19 | 0.68 | 0.11 |
| | Ax + Int[f] | 0.64 | 0.65 | 0.64 | -0.29 | 0.03 | 0.50 | 111 | 21 | 0.68 | 0.11 |
| 2 Ile | *Exp* | *0.57* | *0.60* | *0.61* | *-0.36* | *0.05* | *0.60* | *80* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.24 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 80 | | | 0.24 |
| | Iso + Int | 0.60 | 0.61 | 0.60 | -0.28 | 0.05 | 0.53 | | 19 | 0.73 | 0.08 |
| | Ax + Int | 0.60 | 0.61 | 0.60 | -0.28 | 0.05 | 0.53 | 80 | 18 | 0.73 | 0.08 |
| 3 Cys[g] | *Exp* | | | | *-0.23* | *0.07* | *0.58* | *91* | | | |
| | IsoRigid | | | | -0.31 | 0.04 | 0.57 | | | | 0.06 |
| | Ax Rigid | | | | -0.31 | 0.04 | 0.57 | 91 | | | 0.06 |
| | Iso + Int | | | | -0.26 | 0.07 | 0.57 | | 167 | 0.73 | 0.03 |
| | Ax + Int | | | | -0.26 | 0.07 | 0.56 | 91 | 125 | 0.66 | 0.03 |
| 4 Arg | *Exp* | *0.59* | *0.58* | *0.57* | *-0.47* | *0.04* | *0.63* | *82* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.24 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 82 | | | 0.24 |
| | Iso + Int | 0.57 | 0.58 | 0.57 | -0.29 | 0.04 | 0.52 | | 26 | 0.77 | 0.15 |
| | Ax + Int | 0.57 | 0.58 | 0.57 | -0.29 | 0.04 | 0.52 | 82 | 25 | 0.77 | 0.15 |
| 5 Cys | *Exp* | *0.56* | *0.60* | *0.63* | *0.39* | *0.06* | *0.67* | *79* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.26 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 79 | | | 0.26 |
| | Iso + Int | 0.61 | 0.62 | 0.61 | -0.27 | 0.06 | 0.55 | | 13 | 0.72 | 0.14 |
| | Ax + Int | 0.61 | 0.62 | 0.61 | -0.27 | 0.06 | 0.55 | 79 | 13 | 0.73 | 0.13 |
| 6 Ile | *Exp* | *0.54* | *0.56* | *0.56* | *-0.38* | *0.13* | *0.65* | *67* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.20 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.32 | 0.03 | 0.56 | 67 | | | 0.20 |
| | Iso + Int | 0.56 | 0.57 | 0.56 | -0.23 | 0.10 | 0.59 | | 2 | 0.80 | 0.12 |
| | Ax + Int | 0.55 | 0.57 | 0.56 | -0.21 | 0.12 | 0.60 | 67 | 2 | 0.80 | 0.13 |
| 7 Cys | *Exp* | *0.53* | *0.57* | *0.57* | *-0.35* | *0.12* | *0.61* | *86* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.19 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 86 | | | 0.19 |
| | Iso + Int | 0.56 | 0.57 | 0.56 | -0.23 | 0.10 | 0.59 | | 1 | 0.79 | 0.10 |
| | Ax + Int | 0.56 | 0.57 | 0.56 | -0.23 | 0.10 | 0.59 | 86 | 1 | 0.79 | 0.09 |
| 8 Gly | *Exp* | *0.55* | *0.57* | *0.63* | *-0.30* | *0.09* | *0.62* | *87* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.23 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 87 | | | 0.23 |
| | Iso + Int | 0.60 | 0.62 | 0.60 | -0.23 | 0.10 | 0.59 | | 1 | 0.74 | 0.09 |
| | Ax + Int | 0.60 | 0.62 | 0.60 | -0.24 | 0.10 | 0.59 | 87 | 1 | 0.74 | 0.09 |
| 9 Arg | *Exp* | *0.61* | *0.65* | *0.64* | *-0.31* | *0.08* | *0.56* | *85* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.31 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 85 | | | 0.31 |
| | Iso + Int | 0.64 | 0.65 | 0.64 | -0.25 | 0.08 | 0.56 | | 7 | 0.69 | 0.05 |
| | Ax + Int | 0.64 | 0.65 | 0.64 | -0.26 | 0.07 | 0.56 | 85 | 6 | 0.69 | 0.05 |
| 10 Arg[h] | *Exp* | *0.67* | *0.69* | | *-0.29* | *-0.04* | *0.47* | *76* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.32 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 76 | | | 0.32 |
| | Iso + Int | 0.67 | 0.68 | | -0.35 | -0.03 | 0.45 | | 28 | 0.64 | 0.04 |
| | Ax + Int | 0.67 | 0.68 | 0.67 | -0.35 | -0.03 | 0.45 | 76 | 28 | 0.64 | 0.04 |
| 11 Ile | *Exp* | *0.62* | *0.64* | *0.64* | *-0.28* | *-0.07* | *0.56* | *117* | | | |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.32 |
| | Ax Rigid | 0.46 | 0.47 | 0.46 | -0.32 | 0.03 | 0.56 | 117 | | | 0.31 |
| | Iso + Int | 0.63 | 0.64 | 0.63 | -0.35 | -0.03 | 0.45 | | 34 | 0.68 | 0.10 |
| | Ax + Int | 0.63 | 0.64 | 0.63 | -0.34 | -0.03 | 0.44 | 117 | 37 | 0.67 | 0.10 |
| 12 Cys[g] | *Exp* | | | | *-0.21* | *0.09* | *0.51* | *89* | | | |
| | IsoRigid | | | | -0.31 | 0.04 | 0.57 | | | | 0.09 |
| | Ax Rigid | | | | -0.31 | 0.04 | 0.57 | 89 | | | 0.09 |
| | Iso + Int | | | | -0.25 | 0.08 | 0.57 | | 127 | 0.68 | 0.05 |
| | Ax + Int | | | | -0.25 | 0.08 | 0.57 | 89 | 127 | 0.72 | 0.06 |
| 13 Arg | *Exp* | *0.58* | *0.57* | *0.60* | *-0.38* | *0.04* | *0.59* | *91* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.22 |
| | Ax Rigid | 0.46 | 0.46 | 0.45 | -0.31 | 0.04 | 0.57 | 91 | | | 0.22 |
| | Iso + Int | 0.59 | 0.60 | 0.59 | -0.29 | 0.04 | 0.52 | | 22 | 0.74 | 0.09 |
| | Ax + Int | 0.59 | 0.60 | 0.59 | -0.29 | 0.04 | 0.52 | 91 | 20 | 0.74 | 0.09 |
| 14 Cys | *Exp* | *0.56* | *0.59* | *0.59* | *-0.39* | *0.06* | *0.65* | *101* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.23 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 101 | | | 0.23 |
| | Iso + Int | 0.57 | 0.59 | 0.58 | -0.26 | 0.07 | 0.56 | | 13 | 0.77 | 0.12 |
| | Ax + Int | 0.57 | 0.59 | 0.58 | -0.26 | 0.07 | 0.56 | 101 | 12 | 0.77 | 0.12 |
| 15 Ile | *Exp* | *0.54* | *0.55* | *0.58* | *-0.38* | *0.13* | *0.64* | *114* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.20 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.32 | 0.03 | 0.56 | 114 | | | 0.20 |
| | Iso + Int | 0.55 | 0.56 | 0.55 | -0.23 | 0.10 | 0.59 | | 1 | 0.81 | 0.12 |
| | Ax + Int | 0.55 | 0.56 | 0.55 | -0.21 | 0.12 | 0.60 | 114 | 2 | 0.81 | 0.13 |
| 16 Cys | *Exp* | *0.52* | *0.58* | *0.59* | *-0.25* | *0.07* | *0.62* | *98* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.20 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 98 | | | 0.20 |
| | Iso + Int | 0.55 | 0.56 | 0.55 | -0.25 | 0.08 | 0.56 | | 13 | 0.80 | 0.06 |
| | Ax + Int | 0.55 | 0.56 | 0.55 | -0.25 | 0.08 | 0.57 | 98 | 11 | 0.80 | 0.06 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 17 Gly | *Exp* | *0.61* | *0.58* | *0.61* | *-0.32* | *0.08* | *0.65* | *94* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.26 |
| | Ax Rigid | 0.46 | 0.47 | 0.45 | -0.31 | 0.04 | 0.57 | 94 | | | 0.26 |
| | Iso + Int | 0.61 | 0.62 | 0.61 | -0.27 | 0.06 | 0.55 | | 13 | 0.72 | 0.09 |
| | Ax + Int | 0.61 | 0.62 | 0.61 | -0.27 | 0.06 | 0.55 | 94 | 12 | 0.73 | 0.09 |
| 18 Arg | *Exp* | *0.60* | *0.68* | *0.71* | *-0.25* | *0.04* | *0.44* | *127* | | | |
| | IsoRigid | 0.46 | 0.47 | 0.46 | -0.31 | 0.04 | 0.57 | | | | 0.38 |
| | Ax Rigid | 0.46 | 0.47 | 0.46 | -0.34 | 0.02 | 0.56 | 127 | | | 0.38 |
| | Iso + Int | 0.62 | 0.63 | 0.62 | -0.29 | 0.04 | 0.52 | | 18 | 0.70 | 0.12 |
| | Ax + Int | 0.62 | 0.63 | 0.63 | -0.27 | 0.04 | 0.50 | 127 | 26 | 0.68 | 0.11 |
| RMSD[i] | IsoRigid | 0.50 | 0.58 | 0.65 | 0.20 | 0.16 | 0.20 | | | | |
| | Ax Rigid | 0.50 | 0.58 | 0.65 | 0.21 | 0.16 | 0.19 | | | | |
| | Iso + Int | 0.12 | 0.09 | 0.13 | 0.29 | 0.05 | 0.21 | | | | |
| | Ax + Int | 0.12 | 0.09 | 0.13 | 0.29 | 0.04 | 0.21 | | | | |

[a] Abbreviations used: Exp, experimental data; IsoRigid, isotropic rigid; Ax Rigid, axial rigid; Iso + Int, isotropic with internal motion, Ax + Int, axial with internal motion.

[b] $RMSD = \sqrt{\sum(T_1 exp - T_1 calc)^2 + \sum[0.5(NOEexp - NOEcalc)^2]}$

RMSD is the root mean square deviation between the experimental and fitted (calc) $T_1$ and NOE values. The NOE deviations were weighted by 50% because of their intrinsically higher errors compared to the $T_1$ values.

[c] For isotropic rigid motion, the overall correlation time, $\tau_0 = 1.07$ ns.

[d] For axial rigid motion, the overall correlation time, $\tau_0 = 1.06$ ns and the $D_{ratio} = 0.90$.

[e] For isotropic with internal motion, the overall correlation time, $\tau_0 = 1.13$ ns.

[f] For axial with internal motion, the overall correlation time, $\tau_0 = 1.16$ ns and the $D_{ratio} = 1.27$.

[g] The $^{15}N$ HSQC peaks for Cys3 and Cys12 were overlapped with those of Ile6 and Ile15 and a satisfactory exponential fit could not be obtained to determine $T_1$.

[h] Broadening of the Arg10 NH peak resulted in a poor exponential fit so Arg10 $T_1$ was excluded from the analysis.

[i] $RMSD = \sqrt{\sum(\exp - calc)^2}$

RMSD is the root mean square deviation between the experimental and fitted (calc) $T_1$ and NOE values calculated over all the residues at each field strength.

**Supplementary Table S5: Fitted parameters and errors using an in-house spreadsheet.**

| Model | Residue(s) | $\tau_0$ (ps) | s.d. | $D_{ratio}$ | s.d. | $\tau_i$ (ps) | s.d. | $S^2$ | s.d. |
|---|---|---|---|---|---|---|---|---|---|
| *IsoRigid* | | | | | | | | | |
| | All | 1.05 | 0.004 | | | | | | |
| *Ax Rigid* | | | | | | | | | |
| | All | 1.08 | NA | 2.44 | NA | | | | |
| | All | 1.02 | 0.03 | 0.87 | 0.07 | | | | |
| *Iso + Int* | | | | | | | | | |
| | All | 1.09 | 0.007 | | | | | | |
| | 1 Gly | | | | | 2.45 | 3.82 | 0.71 | 0.03 |
| | 2 Ile | | | | | 6.15 | 3.37 | 0.76 | 0.01 |
| | 3 Cys | | | | | 24.92 | 16.94 | 0.93 | 0.15 |
| | 4 Arg | | | | | 17.56 | 8.43 | 0.77 | 0.02 |
| | 5 Cys | | | | | 1.34 | 3.10 | 0.77 | 0.01 |
| | 6 Ile | | | | | 0.00 | 0.00 | 0.82 | 0.02 |
| | 7 Cys | | | | | 0.00 | 0.00 | 0.82 | 0.01 |
| | 8 Gly | | | | | 1.00 | 2.94 | 0.78 | 0.01 |
| | 9 Arg | | | | | 2.44 | 1.72 | 0.72 | 0.01 |
| | 10 Arg | | | | | 18.10 | 10.10 | 0.66 | 0.02 |
| | 11 Ile | | | | | 11.72 | 7.01 | 0.71 | 0.01 |
| | 12 Cys | | | | | 24.41 | 13.39 | 0.96 | 0.15 |
| | 13 Arg | | | | | 11.55 | 7.45 | 0.8 | 0.01 |
| | 14 Cys | | | | | 3.62 | 4.01 | 0.77 | 0.02 |
| | 15 Ile | | | | | 0.26 | 0.76 | 0.82 | 0.01 |
| | 16 Cys | | | | | 0.00 | 0.00 | 0.81 | 0.01 |
| | 17 Gly | | | | | 0.00 | 0.00 | 0.76 | 0.01 |
| | 18 Arg | | | | | 10.11 | 3.46 | 0.67 | 0.02 |

**Supplementary Table S6: Fitted parameters and errors using MODELFREE.**

| Model | Residue(s) | $\tau_0$ (ps) | s.d. | $D_{ratio}$ | s.d. | $\tau_i$ (ps) | s.d. | $S^2$ | s.d. |
|---|---|---|---|---|---|---|---|---|---|
| *IsoRigid* | | | | | | | | | |
| | All | 1.07 | 0.000 | | | | | | |
| *Ax Rigid* | | | | | | | | | |
| | All | 1.06 | 0.002 | 0.90 | 0.01 | | | | |
| *Iso + Int* | | | | | | | | | |
| | All | 1.13 | 0.002 | | | | | | |
| | 1 Gly | | | | | 18.91 | 1.65 | 0.68 | 0.02 |
| | 2 Ile | | | | | 18.52 | 1.01 | 0.73 | 0.01 |
| | 3 Cys | | | | | 166.56 | 185.00 | 0.73 | 0.29 |
| | 4 Arg | | | | | 26.17 | 1.84 | 0.77 | 0.01 |
| | 5 Cys | | | | | 13.09 | 1.16 | 0.72 | 0.01 |
| | 6 Ile | | | | | 1.70 | 2.01 | 0.80 | 0.01 |
| | 7 Cys | | | | | 1.04 | 1.19 | 0.79 | 0.00 |
| | 8 Gly | | | | | 1.11 | 1.25 | 0.74 | 0.01 |
| | 9 Arg | | | | | 7.21 | 0.52 | 0.69 | 0.01 |
| | 10 Arg | | | | | 27.95 | 2.18 | 0.64 | 0.01 |
| | 11 Ile | | | | | 34.06 | 1.63 | 0.68 | 0.01 |
| | 12 Cys | | | | | 127.38 | 178.02 | 0.68 | 0.32 |
| | 13 Arg | | | | | 21.97 | 1.78 | 0.74 | 0.01 |
| | 14 Cys | | | | | 12.68 | 2.24 | 0.77 | 0.01 |
| | 15 Ile | | | | | 1.44 | 1.89 | 0.81 | 0.01 |
| | 16 Cys | | | | | 12.99 | 2.03 | 0.80 | 0.01 |
| | 17 Gly | | | | | 13.35 | 1.00 | 0.72 | 0.01 |
| | 18 Arg | | | | | 17.71 | 1.78 | 0.70 | 0.02 |
| *Ax + Int* | | | | | | | | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| All | 1.16 | 0.009 | | | | | | |
| All | | | 1.24 | 0.07 | | | | |
| 1 Gly | | | | | 21.10 | 1.91 | 0.68 | 0.02 |
| 2 Ile | | | | | 17.91 | 0.94 | 0.73 | 0.01 |
| 3 Cys | | | | | 124.61 | 176.66 | 0.66 | 0.31 |
| 4 Arg | | | | | 24.88 | 1.82 | 0.77 | 0.01 |
| 5 Cys | | | | | 12.60 | 1.09 | 0.73 | 0.01 |
| 6 Ile | | | | | 1.61 | 2.09 | 0.80 | 0.01 |
| 7 Cys | | | | | 1.00 | 1.20 | 0.79 | 0.00 |
| 8 Gly | | | | | 0.83 | 1.10 | 0.74 | 0.01 |
| 9 Arg | | | | | 6.39 | 0.57 | 0.69 | 0.01 |
| 10 Arg | | | | | 27.92 | 2.30 | 0.64 | 0.01 |
| 11 Ile | | | | | 36.97 | 1.95 | 0.67 | 0.01 |
| 12 Cys | | | | | 127.37 | 177.14 | 0.72 | 0.30 |
| 13 Arg | | | | | 19.99 | 1.78 | 0.74 | 0.30 |
| 14 Cys | | | | | 11.79 | 2.33 | 0.77 | 0.01 |
| 15 Ile | | | | | 1.60 | 2.05 | 0.81 | 0.01 |
| 16 Cys | | | | | 11.22 | 1.96 | 0.80 | 0.01 |
| 17 Gly | | | | | 11.66 | 1.04 | 0.73 | 0.01 |
| 18 Arg | | | | | 26.09 | 3.00 | 0.68 | 0.02 |