# A rigorous and efficient method to reweight very large conformational ensembles using average experimental data and to determine their relative information content

## Supporting Information

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**Table S1A**: Backbone RDC ($^1D_{NH}$, $^1D_{C\alpha H\alpha}$, $^1D_{C\alpha C'}$) and *J*-coupling ($^3J_{HNH\alpha}$, $^3J_{H\alpha N}$) data (in Hz) of the isotope-labeled EGAAWAASS peptide

| Residue | $^3J_{H\alpha N}$ | Err.[a)] | $^3J_{H\alpha HN}$ | Err.[b)] | $^1D_{NH}$ | Err. | $^1D_{C\alpha H\alpha}$ | Err. | $^1D_{C\alpha C'}$ | Err. |
|---|---|---|---|---|---|---|---|---|---|---|
| E1 | | | | | | | 12.95 | 0.46 | -0.59 | 0.11 |
| G2 | -0.49 | 0.16 | | | -5.4 | 0.15 | | | -1.55 | 0.11 |
| A3 | | | 6.05 | 0.3 | -1.26 | 0.15 | 11.5 | 0.46 | -0.67 | 0.11 |
| A4 | -0.54 | 0.16 | 5.95 | 0.3 | -5.22 | 0.15 | 21.42 | 0.46 | -0.94 | 0.11 |
| W5 | -0.53 | 0.16 | 6.44 | 0.3 | -0.91 | 0.15 | -9.37 | 0.46 | -1.49 | 0.2 |
| A6 | | | 6.53 | 0.3 | 2.33 | 0.15 | 10.01 | 0.46 | -0.55 | 0.11 |
| A7 | -0.39 | 0.16 | 5.93 | 0.3 | -2.88 | 0.15 | 15.01 | 0.46 | -0.3 | 0.11 |
| S8 | -0.39 | 0.16 | 6.98 | 0.3 | -8.37 | 0.15 | 15.73 | 0.46 | -1.44 | 0.11 |
| S9 | | | 7.16 | 0.3 | -3.78 | 0.15 | | | | |

[a)]For comparison, the RMSD between experimental $^3J_{H\alpha N}$-couplings and values back-calculated from an x-ray structure was 0.13 Hz using Karplus parameters determined by Löhr et al.[1]

[b)]For comparison, the RMSD between the experimental $^3J_{HNH\alpha}$-couplings and values back-calculated from a structural ensemble is 0.36 Hz using Karplus parameters determined by Vögeli et al.[2]

**Table S1B:** Side chain $^3J_{NC\gamma}$ and $^3J_{C'C\gamma}$ scalar coupling constants (in Hz) of W5 in the EGAAWAASS peptide

| | *J* | Err. |
|---|---|---|
| $^3J_{C'C\gamma}$ | 1.59 | 0.1 |
| $^3J_{NC\gamma}$ | 1.21 | 0.1 |

Using these coupling constants and respective Karplus parameters,[3] the populations of the $\chi_1$ +60˚, +180˚ and -60˚ rotamers are determined as 0.221, 0.464, and 0.312, respectively. Details of this calculation are given in Vajpai et al.[4]

**Table S1C:** Chemical shifts (in ppm) determined for the EGAAWAASS peptide[a)]

| | $H^N$ | N | $H^\alpha$ | $C^\alpha$ | C' | $H^\beta$ | $C^\beta$ |
|---|---|---|---|---|---|---|---|
| E1 | | | 4.103 | 55.83 | 173.15 | 2.152 | 29.99 |
| G2 | 8.780 | 111.42 | 4.034[b] | 45.12 | 173.46 | | |
| A3 | 8.353 | 124.31 | 4.285 | 52.35 | 177.72 | 1.277 | 19.31 |
| A4 | 8.344 | 123.67 | 4.287 | 52.68 | 177.58 | 1.361 | 19.07 |
| W5 | 8.008 | 119.98 | 4.612 | 57.37 | 175.80 | 3.308[b)] | 29.50 |
| A6 | 7.833 | 126.18 | 4.224 | 52.04 | 176.69 | 1.247 | 19.73 |
| A7 | 8.055 | 123.48 | 4.241 | 52.49 | 177.78 | 1.429 | 19.37 |
| S8 | 8.283 | 115.37 | 4.511 | 58.27 | 173.82 | 3.930[b] | 64.13 |
| S9 | 8.024 | 122.84 | | 59.91 | 178.50 | | |

[a)]Chemical shift assignments were derived from a set of standard HNCO, HNCA, CBCACONH, and HBHACONH experiments. $^1$H, $^{15}$N and $^{13}$C chemical shifts are referenced

relative to the frequency of the $^{2}H$ lock resonance of water.
[b)]Methylene resonances overlap.

**Figure S2**

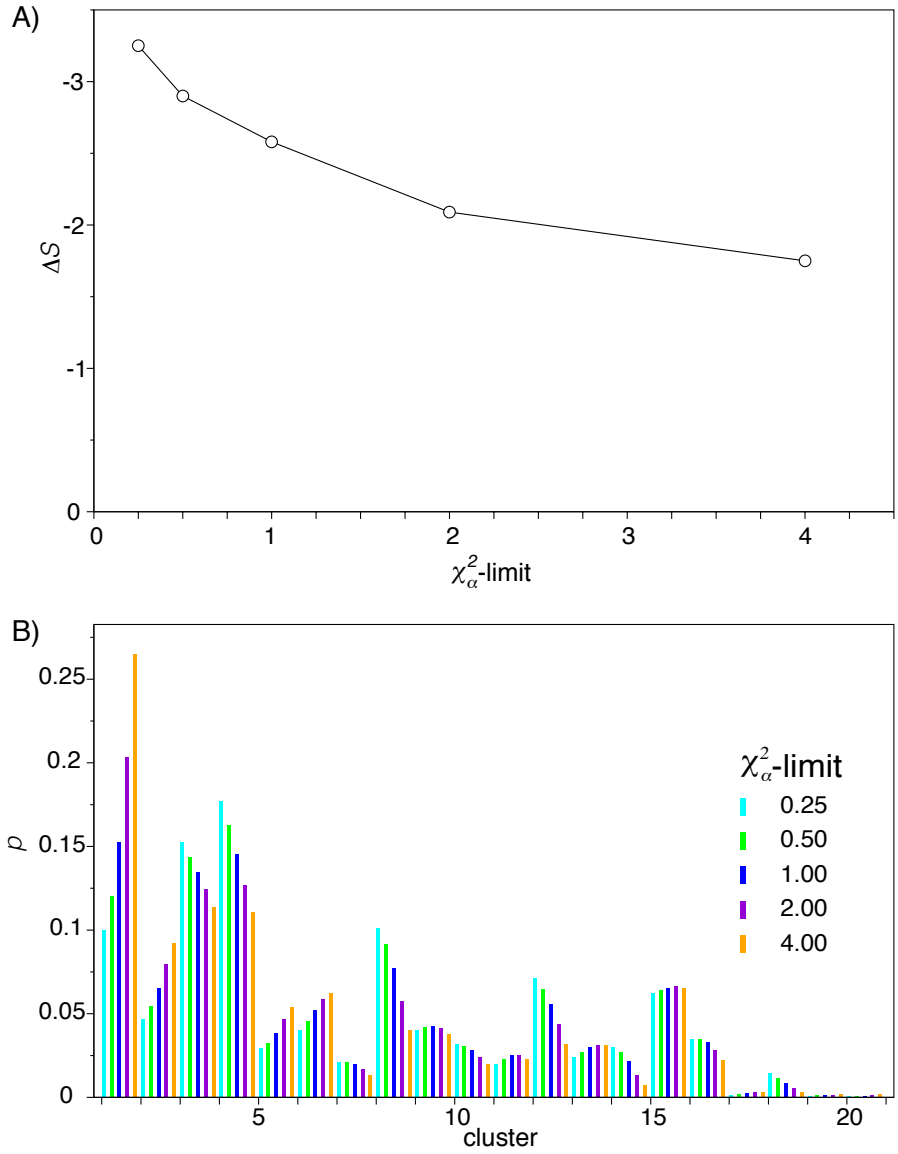


Figure S2: Analysis of the 35000 conformations from the MD conformations of the EGAAWAASS peptide with different $\chi^2_\alpha$-limits. A) The reduction in total entropy $\Delta S$ for $\chi^2_\alpha$-limits of the backbone RDC and *J*-coupling constraints ranging from 0.25 to 4.0. B) Populations of the 20 clusters calculated with $\chi^2_\alpha$-limits ranging from 0.25 to 4.0.

**References**


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