Supporting Information

Details about the SECONDA analysis and SECONDA based selection of experimental data

In order to quantify the similarity of structure and dynamics across the different alignment media (homogeneity of RDC data), a SECONDA analysis is applied (Hus and Brüschweiler, 2002; Hus et al., 2003). The SECONDA method analyzes the covariance matrix constructed of all RDC data obtained under different alignment conditions. It performs a principal component analysis (PCA) of the RDC covariance matrix, which is mathematically equivalent to a singular value decomposition (SVD) of the RDC matrix. The singular values are sorted according to decreasing size. All structural and dynamic information is contained in the first five singular values, since dipolar couplings are a second rank symmetric tensor interaction and hence reside in a linear 5-dimensional space. Accordingly, only noise, systematic errors, and structural and dynamic heterogeneity may cause the 6th and higher singular values to differ from zero. The ratio of the 5th and 6th singular values (called “SECONDA gap” in this work) is a measure of the homogeneity of RDC data and the magnitude of noise. The larger the SECONDA gap, the more self-consistent are the RDC data in the different alignment media.

Since there is no straightforward way to treat missing entries in the RDC covariance matrix, a specific residue can only be considered if experimental data for this residue are available in all selected alignment media (compare (Hus et al., 2003), Scenario I). All experimental RDCs are normalized before the analysis by division through the largest absolute RDC value in each
medium. For D36M, the SECONDA gap was 5.66 with experimental data available for 21 residues in all media.

Starting from these 36 NH RDC data sets, a subset was selected that maximizes the SECONDA gap by reducing the number of data sets and number of amino acids, with the restraint of having a 5th EV of the F matrix with a value larger than 1 (see below).

In a Monte Carlo search that randomly removed amino acids and alignment media in order to maximize the SECONDA gap, a maximum SECONDA gap of 15.18 could be obtained with the alignment media A 2, 4, 9-10, 13-16, 19-20, 22-29, 32-36 out of D36M and the amino acids 2, 5, 7, 11, 14, 25, 27, 32, 33, 36, 40, 44, 49, 51, 55, 58, 63, 66 and 68. This subset of 23 data sets will be called D23M in the following. Considering all residues for which experimental data were available (36 residues) the SECONDA gap was 6.81 after normalization. For comparison, selecting out of the 36 residues the 21 residues that were used for D36M gives a SCONDA gap of 8.69. These rather large SECONDA gaps indicate a highly homogenous behaviour of structure and dynamics across all alignment media contributing to D36M and even more so for D23M.
Selection of RDC data for alignment tensor calculation, Completeness of sampling

To ensure an adequate sampling of the three principal axes of the alignment tensor, an eigenvalue analysis of the matrix

\[ C = B^T B \]

where \( B = (e_1, e_2, \ldots, e_N) \) is the 3xN matrix containing the normalized NH vectors \( e_k \) of the average structure, is performed and the diagonalized matrix \( D = (d(1), d(2), d(3)) \) is obtained that contains the three eigenvalues of \( C \) sorted according to magnitude (see Prompers and Brüschweiler, 2002)).

The ratio \( r \) of the first and third eigenvalue of \( D \) as well as the asymmetry \( a \) defined below are a measure for the goodness of directional sampling:

\[
    r = \sqrt{\frac{d(1)}{d(3)}}
\]

\[
    a = \frac{d(2) - d(3)}{d(1)}
\]

In the ideal case of complete and homogeneous sampling, all eigenvalues of \( D \) are equal to 1, and the ratio \( r = 1 \) and the asymmetry \( a = 0 \).

The reduced NH vector set (number of residues \( N = 49 \)) after four runs of SCRM gives a ratio \( r = 2.17 \) and an asymmetry of \( a = 0.32 \) for the procedure applied on D36M and \( r = 2.01 \) and \( a = 0.28 \) for D23M (\( N = 48 \)). For comparison, the best possible benchmarks are \( r = 1.61 \) and \( a = 0.22 \) when all possible NH vectors (\( N = 68 \)) are used for the analysis. Using NH vectors of secondary
structure elements only (N=40) gives r=2.55 and a=0.22 which is slightly better with respect to asymmetry but significantly worse for r compared to the dynamic selections.

With r and a, we measure the completeness and homogeneity of the sampling of the orientations. For a successful RDC based model free analysis the alignment tensors also need to homogeneously and completely sample the five dimensional space. A measure for completeness is the 5th eigenvalue and the condition number of the F-Matrix (see above). This is an empirical value without physical meaning, but compared to other experimental data sets it gives a first impression of the completeness of RDC-data. The 5th EV of the F-matrix is 1.02 for D23M and 1.31 for D36M, the condition numbers are 6.57 for D23M and 6.28 for D36M. This compares favourably with earlier analyses in which the condition numbers were also between 6 and 7 (Peti et al., 2002) (Lakomek et al., 2006; Lakomek et al., 2005).

**Alternative way of estimating the inhomogeneity on the NH rdc's of D23M**

The RDCs $D_{ij}$ back-calculated from the model-free derived second order spherical harmonics contain dynamic information and are noise-free by definition. Gaussian noise has been added to these data until they yield a SECONDA gap of approximately 6.8, namely $6.5 \pm 0.5$. We found that Gaussian noise of $\sigma = 0.22$ Hz on the RDCs back-calculated for D23M led to this SECONDA gap of $6.5 \pm 0.5$. Based on this analysis the inhomogeneity for data set D23M is estimated to be around 0.22 Hz.
RDC-based order parameters $S_{rdc}^2$

The following order parameters $S_{rdc}^2$ are obtained using the experimental NH RDC data collection D23M. The first line is the residue number, second line the order parameter $S_{rdc}^2$, third the error on the $S_{rdc}^2$ values propagated from the experimental error $\sigma_{exp}^j = 0.3$ Hz and fourth line the error on the $S_{rdc}^2$ propagated from the experimental plus model error $\sigma_{j}^{rmsd} = rmsd(rdc, j)$ (derived using the RDC-rmsd as the input error for the SCRM analysis).

Table S1:

| #  | $S_{rdc}^2$ | Exp. Err. | +Me. | Err. |
|----|-------------|-----------|------|------|
| 1  | n           | n         | n    | n    |
| 2  | 0.85        | 0.06      | 0.06 |      |
| 3  | 0.68        | 0.07      | 0.07 |      |
| 4  | 0.79        | 0.06      | 0.10 |      |
| 5  | 0.75        | 0.04      | 0.04 |      |
| 6  | 0.78        | 0.04      | 0.04 |      |
| 7  | 0.64        | 0.04      | 0.04 |      |
| 8  | 0.67        | 0.04      | 0.06 |      |
| 9  | n           | n         | n    | n    |
| 10 | n           | n         | n    | n    |
| 11 | 0.45        | 0.02      | 0.02 |      |
| 12 | 0.64        | 0.05      | 0.07 |      |
| 13 | 0.68        | 0.03      | 0.03 |      |
| 14 | 0.78        | 0.05      | 0.05 |      |
| 15 | 0.72        | 0.11      | 0.11 |      |
| 16 | n           | n         | n    | n    |
| 17 | 0.86        | 0.06      | 0.06 |      |
| 18 | 0.77        | 0.04      | 0.04 |      |
| 19 | n           | n         | n    | n    |
| 20 | 0.55        | 0.05      | 0.05 |      |
| 21 | 0.86        | 0.05      | 0.05 |      |
| 22 | n           | n         | n    | n    |
| 23 | 0.80        | 0.04      | 0.04 |      |
|   |   |   |   |
|---|---|---|---|
| 24 | n | n | n |
| 25 | 0.83 | 0.05 | 0.05 |
| 26 | n | n | n |
| 27 | 0.82 | 0.04 | 0.04 |
| 28 | 0.85 | 0.04 | 0.06 |
| 29 | 0.73 | 0.04 | 0.04 |
| 30 | 0.77 | 0.04 | 0.04 |
| 31 | n | n | n |
| 32 | 0.84 | 0.04 | 0.04 |
| 33 | 0.76 | 0.04 | 0.04 |
| 34 | 0.73 | 0.04 | 0.04 |
| 35 | 0.82 | 0.04 | 0.04 |
| 36 | 0.76 | 0.04 | 0.04 |
| 37 | n | n | n |
| 38 | n | n | n |
| 39 | n | n | n |
| 40 | 0.67 | 0.03 | 0.03 |
| 41 | 0.80 | 0.03 | 0.03 |
| 42 | 0.69 | 0.06 | 0.06 |
| 43 | 0.77 | 0.06 | 0.08 |
| 44 | 0.75 | 0.03 | 0.03 |
| 45 | 0.80 | 0.06 | 0.06 |
| 46 | n | n | n |
| 47 | 0.77 | 0.05 | 0.05 |
| 48 | 0.59 | 0.03 | 0.03 |
| 49 | 0.72 | 0.04 | 0.04 |
| 50 | 0.59 | 0.03 | 0.08 |
| 51 | 0.74 | 0.07 | 0.07 |
| 52 | 0.69 | 0.03 | 0.06 |
| 53 | n | n | n |
| 54 | 0.69 | 0.03 | 0.03 |
| 55 | 0.77 | 0.05 | 0.05 |
| 56 | 0.72 | 0.04 | 0.06 |
| 57 | n | n | n |
| 58 | 0.87 | 0.08 | 0.08 |
| 59 | 0.81 | 0.04 | 0.04 |
| 60 | 0.80 | 0.03 | 0.03 |
| 61 | 0.90 | 0.04 | 0.04 |
| 62 | 0.55 | 0.01 | 0.02 |
| 63 | 0.79 | 0.03 | 0.03 |
| 64 | 0.88 | 0.05 | 0.07 |
| 65 | 0.66 | 0.04 | 0.08 |
| 66 | 0.87 | 0.06 | 0.06 |
| 67 | 0.82 | 0.04 | 0.04 |
| 68 | 0.80 | 0.04 | 0.04 |
| 69 | n | n | n |
| 70 | 0.70 | 0.04 | 0.04 |
| #  | $s_n^2$ | Exp. Err. | Err. | $\text{Exp.} + \text{Me.}$ |
|----|--------|-----------|------|---------------------------|
| 1  | n      | n         | n    |                           |
| 2  | 0.89   | 0.05      | 0.08 |                           |
| 3  | 0.75   | 0.04      | 0.06 |                           |
| 4  | 0.73   | 0.03      | 0.07 |                           |
| 5  | 0.76   | 0.04      | 0.06 |                           |
| 6  | 0.79   | 0.03      | 0.05 |                           |
| 7  | 0.65   | 0.03      | 0.07 |                           |
| 8  | 0.67   | 0.04      | 0.10 |                           |
| 9  | n      | n         | n    |                           |
| 10 | n      | n         | n    |                           |
| 11 | 0.45   | 0.02      | 0.05 |                           |
| 12 | 0.70   | 0.05      | 0.10 |                           |
| 13 | 0.68   | 0.04      | 0.07 |                           |
| 14 | 0.78   | 0.04      | 0.04 |                           |
| 15 | 0.74   | 0.06      | 0.06 |                           |
| 16 | 0.77   | 0.06      | 0.06 |                           |
| 17 | 0.83   | 0.05      | 0.05 |                           |
| 18 | 0.80   | 0.04      | 0.08 |                           |
| 19 | n      | n         | n    |                           |
| 20 | 0.59   | 0.05      | 0.11 |                           |
| 21 | 0.78   | 0.04      | 0.05 |                           |
| 22 | n      | n         | n    |                           |
| 23 | 0.83   | 0.04      | 0.08 |                           |
| 24 | n      | n         | n    |                           |
| 25 | 0.86   | 0.04      | 0.06 |                           |

n= no data available

Table S2:

|        | 26  | 27  | 28  | 29  | 30  | 31  | 32  | 33  | 34  | 35  | 36  | 37  |
|--------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|        | Exp. |     |     |     |     |     |     |     |     |     |     |     |
|        | 0.78 | 0.82| 0.82| 0.78| 0.79| 0.78| 0.85| 0.75| 0.75| 0.64| 0.77| 0.77|
|        | 0.06 | 0.04| 0.04| 0.06| 0.03| 0.04| 0.04| 0.03| 0.03| 0.03| 0.04| 0.04|
|        | 0.08 | 0.04| 0.09| 0.06| 0.06| 0.05| 0.05| 0.08| 0.09| 0.09| 0.07| 0.07|
|        |      |     |     |     |     |     |     |     |     |     |     |     |
Deviation between dynamic average inter-nuclear vector orientations and X-ray and NMR starting structure

Table S3 (D23M):

The inter-nuclear angles $\kappa_j$ enclosed between the dynamic average NH vector orientations and the NH vectors of the starting X-ray structure 1ubi are shown in column 4 (ubi/ubi) for D23M. In column 5 (ubi/1d3z) the same dynamic average NH vector orientations are compared to the 1d3z NMR structure (see also Figure S2c). For comparison, the SCRM analysis was
repeated using the 1d3z NMR structure as starting structure. The resulting $S_{\text{rdc}}^2(NH)$ and $\kappa_j$ are listed in column 2 and 6 (see also Figure S2e). In column 1 the derived $\kappa_j$ using the 1ubi X-ray structure as starting structure are shown again. Since the C-terminal part of ubiquitin (residues 72-76) are highly mobile, these residues have not been considered for the determination of inter-nuclear angles $\kappa_j$.

| residue # | $S_{\text{rdc}}^2 (1\text{ubi})$ | $S_{\text{rdc}}^2 (1d3z)$ | $\kappa$ ubi/ubi | $\kappa$ ubi/1d3z | $\kappa$ 1d3z/1d3z |
|-----------|-------------------------------|-----------------|-----------------|-----------------|-----------------|
| 1         | n                             | n               | n               | n               | n               |
| 2         | 0.85                          | 0.86            | 4.2             | 5.0             | 5.1             |
| 3         | 0.68                          | 0.68            | 7.6             | 1.8             | 2.9             |
| 4         | 0.79                          | 0.81            | 4.6             | 10.8            | 10.1            |
| 5         | 0.75                          | 0.76            | 3.8             | 2.2             | 2.5             |
| 6         | 0.78                          | 0.80            | 10.4            | 2.6             | 2.8             |
| 7         | 0.64                          | 0.62            | 6.3             | 8.8             | 8.8             |
| 8         | 0.67                          | 0.64            | 5.7             | 8.7             | 8.1             |
| 9         | n                             | n               | n               | n               | n               |
| 10        | n                             | n               | n               | n               | n               |
| 11        | 0.45                          | 0.46            | 17.2            | 11.1            | 12.0            |
| 12        | 0.64                          | 0.63            | 9.2             | 3.8             | 3.2             |
| 13        | 0.68                          | 0.68            | 12.8            | 5.2             | 5.7             |
| 14        | 0.78                          | 0.80            | 9.6             | 3.2             | 3.1             |
| 15        | 0.72                          | 0.73            | 7.3             | 2.0             | 0.9             |
| 16        | n                             | n               | n               | n               | n               |
| 17        | 0.86                          | 0.85            | 7.0             | 3.1             | 3.7             |
| 18        | 0.77                          | 0.79            | 9.5             | 0.7             | 1.5             |
| 19        | n                             | n               | n               | n               | n               |
| 20        | 0.55                          | 0.55            | 12.4            | 7.1             | 6.5             |
| 21        | 0.86                          | 0.83            | 3.2             | 2.8             | 3.0             |
| 22        | n                             | n               | n               | n               | n               |
| 23        | 0.80                          | 0.81            | 6.0             | 4.6             | 4.6             |
| 24        | n                             | n               | n               | n               | n               |
| 25        | 0.83                          | 0.84            | 3.9             | 3.0             | 3.0             |
| 26        | n                             | n               | n               | n               | n               |
| 27        | 0.82                          | 0.82            | 3.7             | 2.8             | 2.2             |
| 28        | 0.85                          | 0.85            | 1.8             | 3.2             | 3.2             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 29 | 0.73 | 0.74 | 2.0 | 4.7 | 4.9 |
| 30 | 0.77 | 0.78 | 0.8 | 0.5 | 0.3 |
| 31 | n  | n  | n  | n  | n  |
| 32 | 0.84 | 0.84 | 7.3 | 4.0 | 4.5 |
| 33 | 0.76 | 0.77 | 11.4 | 1.2 | 1.2 |
| 34 | 0.73 | 0.75 | 15.8 | 2.7 | 3.0 |
| 35 | 0.82 | 0.81 | 6.9 | 5.1 | 6.1 |
| 36 | 0.76 | 0.77 | 9.7 | 8.7 | 8.4 |
| 37 | n  | n  | n  | n  | n  |
| 38 | n  | n  | n  | n  | n  |
| 39 | n  | n  | n  | n  | n  |
| 40 | 0.67 | 0.67 | 2.4 | 4.8 | 5.0 |
| 41 | 0.80 | 0.78 | 6.5 | 5.7 | 5.1 |
| 42 | 0.69 | 0.70 | 12.0 | 7.3 | 8.3 |
| 43 | 0.77 | 0.76 | 10.7 | 3.6 | 3.6 |
| 44 | 0.75 | 0.76 | 8.1 | 4.6 | 5.4 |
| 45 | 0.80 | 0.78 | 5.8 | 1.2 | 1.7 |
| 46 | n  | n  | n  | n  | n  |
| 47 | 0.77 | 0.77 | 2.4 | 13.0 | 12.8 |
| 48 | 0.59 | 0.59 | 11.8 | 3.1 | 3.9 |
| 49 | 0.72 | 0.71 | 3.4 | 2.4 | 2.5 |
| 50 | 0.59 | 0.60 | 10.2 | 3.9 | 3.9 |
| 51 | 0.74 | 0.73 | 3.8 | 3.0 | 3.3 |
| 52 | 0.69 | 0.68 | 15.5 | 21.2 | 20.1 |
| 53 | n  | n  | n  | n  | n  |
| 54 | 0.69 | 0.70 | 20.3 | 2.4 | 2.8 |
| 55 | 0.77 | 0.79 | 0.6 | 2.0 | 2.3 |
| 56 | 0.72 | 0.72 | 5.9 | 3.1 | 3.5 |
| 57 | n  | n  | n  | n  | n  |
| 58 | 0.87 | 0.86 | 1.1 | 1.9 | 2.3 |
| 59 | 0.81 | 0.82 | 2.5 | 2.3 | 3.0 |
| 60 | 0.80 | 0.78 | 4.4 | 8.7 | 8.6 |
| 61 | 0.90 | 0.85 | 7.3 | 3.0 | 3.3 |
| 62 | 0.55 | 0.55 | 3.9 | 4.1 | 3.0 |
| 63 | 0.79 | 0.77 | 0.5 | 2.9 | 2.5 |
| 64 | 0.88 | 0.86 | 3.1 | 3.7 | 3.6 |
| 65 | 0.66 | 0.65 | 2.5 | 6.4 | 6.6 |
| 66 | 0.87 | 0.88 | 4.2 | 1.7 | 0.6 |
| 67 | 0.82 | 0.83 | 10.2 | 3.8 | 4.2 |
| 68 | 0.80 | 0.81 | 2.9 | 4.2 | 4.2 |
| 69 | n  | n  | n  | n  | n  |
| 70 | 0.70 | 0.72 | 11.9 | 6.3 | 6.1 |
| 71 | 0.57 | 0.57 | 10.1 | 7.7 | 8.1 |
Table S4: Same as Table S3 but for D36M.

| residue # | $S^2_{red} \text{ (1ubi)}$ | $S^2_{red} \text{ (1d3z)}$ | $\kappa \text{ ubi/ubi}$ | $\kappa \text{ ubi/1d3z}$ | $\kappa \text{ 1d3z/1d3z}$ |
|----------|--------------------------|--------------------------|---------------------|---------------------|---------------------|
| 1        | n                        | n                        | n                   | n                   | n                   |
| 2        | 0.89                     | 0.89                     | 3.7                 | 5.9                 | 5.9                 |
| 3        | 0.75                     | 0.76                     | 7.9                 | 2.2                 | 3.5                 |
| 4        | 0.73                     | 0.71                     | 5.5                 | 12.5                | 11.4                |
| 5        | 0.76                     | 0.78                     | 3.1                 | 1.6                 | 1.6                 |
| 6        | 0.79                     | 0.80                     | 10.8                | 2.5                 | 2.9                 |
| 7        | 0.65                     | 0.64                     | 6.6                 | 8.6                 | 8.3                 |
| 8        | 0.67                     | 0.64                     | 7.7                 | 11.3                | 10.8                |
| 9        | n                        | n                        | n                   | n                   | n                   |
| 10       | n                        | n                        | n                   | n                   | n                   |
| 11       | 0.45                     | 0.45                     | 16.4                | 10.6                | 10.9                |
| 12       | 0.70                     | 0.69                     | 9.4                 | 3.7                 | 3.8                 |
| 13       | 0.68                     | 0.69                     | 12.0                | 4.5                 | 4.9                 |
| 14       | 0.78                     | 0.80                     | 9.5                 | 2.5                 | 2.3                 |
| 15       | 0.74                     | 0.74                     | 7.4                 | 1.8                 | 0.7                 |
| 16       | 0.77                     | 0.77                     | 2.0                 | 2.6                 | 3.5                 |
| 17       | 0.83                     | 0.81                     | 8.3                 | 3.4                 | 3.9                 |
| 18       | 0.80                     | 0.80                     | 9.4                 | 1.6                 | 1.7                 |
| 19       | n                        | n                        | n                   | n                   | n                   |
| 20       | 0.59                     | 0.59                     | 11.3                | 5.6                 | 5.0                 |
| 21       | 0.78                     | 0.77                     | 2.1                 | 2.5                 | 2.7                 |
| 22       | n                        | n                        | n                   | n                   | n                   |
| 23       | 0.83                     | 0.84                     | 6.3                 | 4.9                 | 4.8                 |
| 24       | n                        | n                        | n                   | n                   | n                   |
| 25       | 0.86                     | 0.87                     | 2.0                 | 2.3                 | 2.3                 |
| 26       | 0.78                     | 0.79                     | 3.0                 | 3.6                 | n                   |
| 27       | 0.82                     | 0.82                     | 2.5                 | 1.4                 | 1.0                 |
| 28       | 0.82                     | 0.83                     | 2.3                 | 2.5                 | 2.8                 |
| 29       | 0.78                     | 0.79                     | 1.5                 | 2.8                 | 3.0                 |
| 30       | 0.79                     | 0.79                     | 1.5                 | 1.1                 | 1.4                 |
| 31       | n                        | n                        | n                   | n                   | n                   |
| 32       | 0.85                     | 0.85                     | 6.6                 | 2.5                 | 2.9                 |
| 33       | 0.75                     | 0.77                     | 10.9                | 1.4                 | 1.2                 |
| 34       | 0.75                     | 0.76                     | 16.5                | 3.5                 | 3.7                 |

n= no data available
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 35 | 0.64 | 0.65 | 11.4 | 10.1 | 10.8 |
| 36 | 0.77 | 0.78 | 7.9  | 7.1  | 7.1  |
| 37 | n   | n   | n   | n   | n   |
| 38 | n   | n   | n   | n   | n   |
| 39 | 0.68 | 0.69 | 2.5  | 3.0  | 3.8  |
| 40 | 0.71 | 0.71 | 2.3  | 3.2  | 3.8  |
| 41 | 0.77 | 0.76 | 7.5  | 4.9  | 4.8  |
| 42 | 0.74 | 0.75 | 12.0 | 7.4  | 8.7  |
| 43 | 0.75 | 0.75 | 12.0 | 4.9  | 4.8  |
| 44 | 0.75 | 0.75 | 8.9  | 5.4  | 6.1  |
| 45 | 0.78 | 0.77 | 6.6  | 1.4  | 2.1  |
| 46 | n   | n   | n   | n   | n   |
| 47 | 0.79 | 0.79 | 2.4  | 13.1 | 13.2 |
| 48 | 0.58 | 0.58 | 13.6 | 4.9  | 5.2  |
| 49 | 0.77 | 0.77 | 4.1  | 1.0  | 1.5  |
| 50 | 0.63 | 0.61 | 7.7  | 1.4  | 1.3  |
| 51 | 0.84 | 0.84 | 3.7  | 4.1  | 4.3  |
| 52 | 0.62 | 0.62 | 11.1 | 17.0 | 16.2 |
| 53 | n   | n   | n   | n   | n   |
| 54 | 0.64 | 0.64 | 19.9 | 2.6  | 3.4  |
| 55 | 0.77 | 0.78 | 0.4  | 1.8  | 2.1  |
| 56 | 0.76 | 0.76 | 7.2  | 4.2  | 4.5  |
| 57 | 0.86 | 0.85 | 11.5 | 6.1  | 7.5  |
| 58 | 0.84 | 0.84 | 1.4  | 1.7  | 1.9  |
| 59 | 0.83 | 0.84 | 3.3  | 2.3  | 3.3  |
| 60 | 0.80 | 0.80 | 5.6  | 8.1  | 8.4  |
| 61 | 0.83 | 0.80 | 6.3  | 1.4  | 2.0  |
| 62 | 0.57 | 0.57 | 4.6  | 5.1  | 4.4  |
| 63 | 0.68 | 0.68 | 1.1  | 3.9  | 4.2  |
| 64 | 0.79 | 0.77 | 2.7  | 3.1  | 2.7  |
| 65 | 0.63 | 0.64 | 4.1  | 5.6  | 5.2  |
| 66 | 0.81 | 0.82 | 4.5  | 1.9  | 0.5  |
| 67 | 0.83 | 0.85 | 9.3  | 3.5  | 4.3  |
| 68 | 0.83 | 0.83 | 3.1  | 3.4  | 3.1  |
| 69 | n   | n   | n   | n   | n   |
| 70 | 0.72 | 0.74 | 11.5 | 6.5  | 5.7  |
| 71 | 0.67 | 0.67 | 7.8  | 10.0 | 9.7  |
| 72 | n   | n   | n   | n   | n   |
Estimation of $S_{\text{overall}}^2$

The scaling of the unscaled RDC-based $S_{\text{rdc, unscaled}}^2$ order parameters based on the Lipari-Szabo order parameter $S_{LS}^2$ becomes non-trivial when taking the experimental error $\sigma$ into account. Therefore, we developed a robust statistical scaling method that will be explained in the following. Our main goal is to derive a conservative estimate for the overall scaling factor $S_{\text{overall}}^2$ such that a confidence level $1 - \alpha$ can be provided for the estimated $S_{\text{overall}}^2$.

Let us assume we knew the true RDC-based order parameters $S_{\text{rdc, unscaled, true}}^2$ for the different residues $i$. We will call them $f_i$. They have to be scaled with respect to the known $S_{LS,i}^2$ that will be called $g_i$. The constant overall scaling factor $S_{\text{overall}}^2$ will be called $\lambda$ in the following. First, we define a true underlying scaling factor $\lambda^*$ that is the maximal factor $\lambda$, such that $\lambda f_i \leq g_i$ is fulfilled for all residues $i$:

$$
\lambda^* = \max_{\lambda} \{ \lambda f_i \leq g_i \} = \min_{i=1,...,n} \left\{ \frac{g_i}{f_i} \right\} = \frac{1}{\max_{i=1,...,n} \left\{ \frac{f_i}{g_i} \right\}} = \frac{1}{\max_{i=1,...,n} \left\{ f_i^* \right\}}
$$

with $f_i^* = \frac{f_i}{g_i}$ and $n$ as the number of residues for which both $f_i$ and $g_i$ are available and non-zero.

As explained in detail in the paragraph Error calculation for the SCRM analysis, the effect of the experimental error on the RDCs leads to an error...
\( \sigma_i^2 \) on the derived order parameters \( S_{\text{dc,unscaled},i}^2 \) that will be called \( Y_i \) in the following.

Because the true overall scaling factor \( \lambda^* \) is unknown, it will be estimated by

\[
\hat{\lambda} = \frac{1}{\text{Max}_{i=1,...,n} \{Y_i^*\}} \quad \text{with} \quad Y_i^* = \frac{Y_i}{g_i}.
\]

Now we want to give an upper bound for the true \( \lambda^* \) with a certain classified probability. For that, confidence-levels \( 1 - \alpha \) are used. We ask: What is the probability that our upper bound exceeds the true unknown scaling factor \( \lambda^* \):

\[
P\left( \lambda^* < \hat{\lambda}_\alpha^u \right) = 1 - \alpha ?
\]

Now we show how to determine \( \hat{\lambda}_\alpha^u \) such that the previous equation is fulfilled for a certain confidence level, like e.g.

\[
P\left( \lambda^* < \hat{\lambda}_\alpha^u \right) = 1 - \alpha = 0.95.
\]

Unfortunately, this turned out not be distribution-independent.

Therefore, we considered the distribution function

\[
F_{\text{max}}(b) = P\left( \text{Max}_i Y_i^* - \text{Max}_i f_i^* \leq b \right)
\]

that describes the probability, that the difference between maximum value of the measurement \( Y^* = \frac{Y}{g} \) and the maximum value of the true curve \( f^* \) is smaller than \( b \). Indeed, \( F_{\text{max}}(b) \) is dependent on the true curve \( f^* \) which means, that the problem is not distribution-independent, as mentioned before. In order to overcome this difficulty, let us assume now that the true curve \( f^* \) is close to the curve of measured data \( Y^* \). We assume that the measured order parameter can be
found within a distribution of order parameters with variance $\sigma_i^2$ around the
unknown true order parameter $Y_i = f_i + \varepsilon_i \sigma_i$ (where the error $\varepsilon_i \sigma_i$ is one
element of this distribution).

The propagation of this experimental error is estimated by adding Gaussian
noise on the RDCs and repeating the SCRM analysis $N=1000$ times. That
yields $j=1...1000$ $Y_{ij}^*$ order parameter values for each residue $i$ forming a
distribution with variance $\sigma_i^2$. Accordingly, we have generated new data with
expectation of our experimental vector $Y^* = E Y_j$.

The distribution function is constructed out of the $N$ different $Y_{ij}^*$ curves.

We calculate $N$ times $\text{Max} Y_{ij}^* - \text{Max} f_i^*$ for the different $Y_{ij}^*$ and by this
generate the distribution function $F_{\text{max}}(b)$ (compare Figure S1).

Starting from $1 - \alpha = F_{\text{max}}(b) = P \left( \text{Max} Y_{ij}^* - \text{Max} f_i^* \leq b \right)$ we can invert for the
upper bound $b$. Using the relationship $\lambda^* = \frac{1}{\text{Max} \{ f_i^* \}}$ gives

$$1 - \alpha = F_{\text{max}}(b) = P \left( \frac{1}{\lambda^*} - \frac{1}{\lambda} \leq b \right)$$

which can be transformed into

$$1 - \alpha = P \left( \lambda^* \leq \frac{\frac{1}{\lambda - b}}{\lambda} \right) = P \left( \lambda^* \leq \hat{\lambda}_\alpha \right) .$$
Now we obtain the required confidence bound $\hat{\lambda}_{\alpha}$ for the estimated scaling factor

$$\hat{\lambda}_{\alpha} = \frac{1}{1 - b\frac{1}{\hat{\lambda}}}.$$ 

This means: The probability that the true (unknown) scaling factor $\lambda^*$ is smaller than the upper bound $\hat{\lambda}_{\alpha}$ is $P\left(\lambda^* \leq \hat{\lambda}_{\alpha}\right) = 1 - \alpha$.

Back to our experimental data we calculate the distribution function $F_{\text{max}}(b)$ (compare Figure S1).

For the experimental error $\sigma = 0.3$ Hz. we calculate $\hat{\lambda}_{\alpha} = 0.80$. Which is equivalent to

$$P\left(S_{\text{overall}} \leq 0.89\right) = 0.95.$$ That means that the probability for the true overall scaling factor to be lower than 0.89 is 95% - which is a conservative estimate.

Since our derivation has been based on the assumption that the true curve is close to the curve of measured data points, we tested the stability of our derivation by exchanging the true curve $f^*$ by one of the simulated experimental curves $Y_j^*$ and leaving $b$ unaltered. This has been done $M=200$ times. A slight tendency for an increase in confidence level has been observed with an average confidence level of $\langle 1 - \alpha \rangle = 0.97$. 
This scaling method has been applied to scale RDC-based $S_{rc}^2$ order parameters derived from D36M with respect to the Lipari-Szabo ones $S_{LS}^2$. The confidence level was estimated taking the error propagation of the experimental error on the RDCs of $\sigma_j^{exp} = 0.3$ Hz into account.

If we consider the experimental plus model error estimated from the RDC-rmsd $\sigma_j^{rmsd} = rmsd(rc, j)$, the confidence level is $P(S_{overall} \leq 0.89) = 0.67$.

The derived overall scaling factor is transferred to D23M as well.

**Hypothesis Test**

The results of the scaling method presented above were tested by an independent hypothesis test. It was first applied to test the hypothesis that the $S_{LS}^2$ and $S_{rc}^2$ order parameters (at any scaling) might stem from the same distribution (zero supra-$\tau_e$ motion hypothesis). Practically, this is achieved by the generation of multiple sets of synthetic order parameters, gauss-distributed around the measured $S_{rc}^2$ order parameters with a standard deviation given by the respective uncertainties. The zero supra-$\tau_e$ motion hypothesis was rejected with a confidence of more than 99.999%, indicating significant supra-$\tau_e$ motion. To obtain a scaling estimate, the method successively removes residues that display the most significant supra-$\tau_e$ motion until the zero supra-$\tau_e$ motion hypothesis cannot anymore be rejected with more than 95% confidence. The corresponding scale that optimally scales the remaining SCRM order parameters to the respective $S_{LS}^2$ order
parameters is the suggested scaling factor. Uncertainties in order parameters were estimated both from the experimental error on the RDC's $\sigma_j^{\text{exp}} = 0.3$ Hz and from the average $\sigma_j^{\text{rmsd}} = \text{rmsd}(rdc, j)$ (0.5 Hz), yielding scaling factors $S_{\text{overall}}^2$ of 0.88 and 0.91.

These results corroborate the presence of supra-$\tau_c$ motion and the estimated scaling factor of the first analysis.

**NH RDCs in different alignment media**

The following RDCs (in Hz) have been newly measured for the different alignment conditions A1-A13. Alignment conditions A14-A18 have been taken from a previous work (Lakomek et al., 2006) and A19-A36 from the literature as indicated.

**Table S5:**

| Source Identifier | A1    | A2    | A3    | A4    | A5    | A6    | A7    | A8    |
|-------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| A1-A8             | SCRM  | SCRM  | SCRM  | SCRM  | SCRM  | SCRM  | SCRM  | SCRM  |
| Source            |       |       |       |       |       |       |       |       |
| Identifier        |       |       |       |       |       |       |       |       |
| D23M              |       |       |       |       |       |       |       |       |
| 1                 | n     | n     | n     | n     | n     | n     | n     | n     |
| 2                 | -1.81 | -3.22 | -20.99 | 14.72 | 10.46 | 8.41  | 13.66 | 4.53  |
|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2.25 | 5.07 | 1.11 | -5.68 | -18.17 | -14.13 | -10.97 | -3.32 |
| 4 | 2.13 | 3.67 | 3.16 | -4.61 | -12.90 | -10.20 | -9.20 | -2.59 |
| 5 | -0.89 | -0.94 | 2.62 | -2.28 | -3.99 | -4.13 | -6.90 | -3.46 |
| 6 | -1.91 | -2.77 | -12.16 | -3.23 | 12.32 | 9.76 | -6.72 | -0.36 |
| 7 | -2.01 | -3.18 | -12.17 | 7.10 | 22.04 | 17.48 | 1.33 | -0.46 |
| 8 | n | n | -3.75 | -4.11 | 6.69 | 6.84 | -11.58 | -6.22 |
| 9 | n | n | n | n | n | n | n | n |
| 10 | n | n | n | n | n | n | n | n |
| 11 | -3.47 | -6.76 | -17.91 | 16.49 | 16.71 | 14.21 | 14.45 | 4.12 |
| 12 | -1.50 | n | -12.22 | 1.48 | 21.37 | 17.65 | -5.69 | -1.79 |
| 13 | -1.93 | -2.78 | n | 2.18 | 0.12 | -0.58 | -1.72 | -2.21 |
| 14 | -0.81 | -0.76 | -5.42 | -4.71 | -1.46 | -1.54 | -8.56 | -1.64 |
| 15 | 3.19 | 6.98 | 9.90 | -7.41 | n | n | -12.71 | -4.98 |
| 16 | 0.57 | 1.75 | -10.35 | 1.75 | -6.23 | -4.51 | -1.42 | 0.58 |
| 17 | 2.63 | 5.74 | -10.40 | 4.71 | n | 3.17 | -1.30 | -1.31 |
| 18 | -2.68 | -5.65 | -20.85 | 19.34 | 16.41 | 13.47 | 18.90 | 5.65 |
| 19 | n | n | n | n | n | n | n | n |
| 20 | -3.22 | -6.87 | 9.42 | 11.04 | n | n | 11.52 | n |
| 21 | 2.55 | 5.98 | n | 3.52 | 18.16 | 16.26 | -3.60 | -2.74 |
| 22 | n | n | n | n | n | n | n | -7.86 |
| 23 | -1.78 | -2.78 | -11.93 | -3.28 | n | n | -6.98 | -0.41 |
| 24 | n | n | n | n | n | n | n | n |
| 25 | -2.47 | -4.90 | -18.62 | -3.12 | 10.56 | 8.41 | -1.11 | 4.30 |
| 26 | -2.03 | -2.99 | -10.98 | -2.57 | 10.65 | 7.89 | -5.92 | -0.75 |
| 27 | -1.18 | -1.75 | -16.58 | -4.80 | n | 20.12 | -7.35 | 0.36 |
| 28 | -2.72 | -5.33 | n | -4.39 | 16.18 | 14.77 | -3.20 | 4.34 |
| 29 | -1.64 | -2.67 | -11.78 | -4.37 | 4.40 | 3.25 | -5.53 | 1.14 |
| 30 | -1.92 | -2.79 | -14.93 | -2.79 | 19.07 | 15.99 | -6.54 | -0.16 |
| 31 | -1.13 | -2.32 | -12.75 | -7.25 | n | 18.55 | -6.57 | 1.92 |
| 32 | -2.61 | -5.50 | -19.19 | -3.66 | n | 12.98 | -0.64 | 5.48 |
| 33 | -1.52 | -2.79 | -9.76 | -3.65 | 6.74 | 5.09 | -6.15 | 0.08 |
| 34 | -1.25 | -2.08 | -16.13 | -6.31 | 23.99 | 18.84 | -6.97 | 1.57 |
| 35 | -2.51 | -7.13 | 8.08 | 1.35 | -3.94 | -4.21 | 13.73 | 5.09 |
| 36 | -4.01 | -8.63 | -22.13 | 18.96 | 14.24 | 10.53 | 22.26 | 6.59 |
| 37 | n | n | n | n | n | n | n | n |
| 38 | n | n | n | n | n | n | n | n |
| 39 | 3.78 | 7.51 | 16.55 | -10.06 | -27.45 | -22.09 | -15.74 | -6.54 |
| 40 | -0.54 | -1.56 | 24.71 | 1.59 | -23.04 | -19.67 | 2.07 | -3.38 |
| 41 | 7.26 | 14.30 | 23.30 | -18.55 | -16.55 | -11.88 | -20.24 | -7.00 |
| 42 | 2.00 | 3.77 | -8.39 | -10.76 | n | 18.88 | -11.49 | -0.44 |
| 43 | 2.43 | 5.23 | -12.07 | -8.19 | 22.94 | n | -13.17 | -2.47 |
| 44 | -1.47 | -1.98 | -17.74 | -3.43 | n | n | -6.79 | 0.21 |
| 45 | -2.40 | -3.53 | -14.55 | 6.71 | 24.82 | 20.30 | 1.21 | -0.51 |
| 46 | n | n | n | n | n | n | n | n |
| 47 | -1.83 | -2.96 | -11.26 | -3.52 | n | n | -7.15 | n |
| 48 | -5.15 | -10.39 | -5.53 | 19.21 | 8.91 | 5.59 | 22.38 | 5.54 |
|   | A9  | A10 | A11 | A12  | A13  | A14  | A15  | A16  |
|---|-----|-----|-----|------|------|------|------|------|
| Source | SCRM | SCRM | SCRM | SCRM | SCRM | L2006 | L2006 | L2006 |
| Identifier | A9  | A10 | A11 | A12  | A13  | E1   | E2   | E3   |
| D23M | x   | x   | x   | x    | x    | x    | x    | x    |
| 1   | n   | n   | n   | n    | n    | n    | n    | n    |
| 2   | 11.16 | 7.87 | 14.76 | 17.41 | 17.60 | 15.74 | 2.61  | 6.74  |
| 3   | -13.39 | -7.56 | -13.68 | -12.15 | -12.55 | -11.03 | -3.79 | -2.78 |
| 4   | -14.09 | -8.34 | -17.43 | -11.25 | -10.35 | -10.74 | -0.05 | -2.76 |
| 5   | -18.23 | -8.10 | -16.44 | -11.00 | -7.39 | -7.80 | 3.46  | -1.75 |
| 6   | -12.74 | -7.57 | -14.68 | -9.48 | -5.02 | n    | 4.30  | -1.66 |
| 7   | -13.90 | -2.76 | -4.87 | -1.75 | 2.66  | 3.44  | 6.78  | 2.74  |
| 8   | -26.33 | -6.24 | -13.84 | -12.40 | -17.16 | n    | n    | n    |
| 9   | n   | n   | n   | n    | n    | n    | n    | n    |
| 10  | n   | n   | n   | n    | n    | n    | n    | n    |
|   | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|----|----|----|----|----|----|----|----|
|   |    | -17.41 | -14.33 | -12.51 | -17.59 | -1.09 | -8.94 | 12.84 |
| n | 7.69 | -6.26 | -5.37 | -8.20 | -8.75 | -1.40 | -0.16 | 10.08 |
| n | 7.58 | n | -10.95 | -15.99 | -17.91 | -2.42 | -0.38 | 16.51 |
| n | 16.24 | n | -6.08 | -11.49 | -15.28 | -0.61 | -0.23 | 20.94 |
| n | 14.35 | n | -1.49 | -7.75 | -16.32 | 0.48 | -2.64 | 23.35 |
| n | 19.19 | n | -3.59 | -7.55 | -14.52 | -0.09 | 1.74 | 19.92 |
| n | 16.90 | n | 5.07 | 1.94 | -3.64 | -1.45 | -3.13 | 5.40 |
| n | 6.04 | n | 0.31 | -2.54 | 0.76 | 2.19 | 8.64 | n |
| 19 | n | n | n | n | n | n | n | n |
| 20 | n | n | n | n | n | n | n | n |
| 21 | n | -2.32 | -3.90 | -7.70 | n | n | 25.50 | 6.66 |
| n | -3.71 | -9.07 | -18.30 | -3.02 | n | 26.00 | -7.54 | -11.80 |
| n | -6.88 | -5.64 | -4.93 | 0.90 | n | 27.00 | -9.16 | -9.18 |
| n | 1.41 | -3.92 | 3.71 | 1.76 | n | n | n | n |
| 24 | n | n | n | n | n | n | n | n |
| 25 | 6.56 | -2.24 | -6.57 | 1.47 | -2.90 | 3.02 | -1.66 | -7.66 |
| n | -2.72 | -8.67 | -4.93 | 0.09 | n | n | n | n |
| 26 | -1.39 | -4.32 | -9.16 | -6.56 | n | n | n | n |
| 27 | -1.29 | -3.71 | -4.93 | -2.33 | n | n | n | n |
| 28 | -1.87 | -3.71 | -4.13 | 2.12 | n | n | n | n |
| 29 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 30 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 31 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 32 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 33 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 34 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 35 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 36 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 37 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 38 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 39 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 40 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 41 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 42 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 43 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 44 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 45 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 46 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 47 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 48 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 49 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 50 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 51 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 52 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 53 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 54 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 55 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
| 56 | -1.18 | -3.71 | -3.70 | 2.73 | n | n | n | n |
A17\text{-}A22:

| Pub | A17 | A18 | A19 | A20 | A21 | A22 |
|-----|-----|-----|-----|-----|-----|-----|
| Source | L2006 | L2006 | T2001 | T2001 | T2001 | T2001 |
| Identify | E4 | E5 | DIDC1 | DIDC2 | DIDC3 | DIDC4 |
| D23M | x | x | x |
| 1 | n | n | n | n | n | n |
| 2 | -6.16 | 5.40 | 8.17 | 15.52 | -4.73 | -4.04 |
| 3 | -1.48 | -8.97 | -8.27 | -10.52 | -0.95 | -0.65 |
| 4 | -1.63 | -7.32 | -10.49 | -9.65 | -1.61 | -1.27 |
| 5 | -2.07 | -3.45 | -9.87 | -6.08 | -1.85 | -1.54 |
| 6 | -6.16 | n | -9.15 | -3.85 | -5.21 | -4.28 |
| 7 | -5.59 | 9.92 | -3.70 | 3.40 | -4.97 | -3.94 |
| 8 | n | n | -6.46 | -15.05 | 0.24 | 0.46 |
| 9 | n | n | n | n | n | n |
| 10 | n | n | n | n | n | n |
| 11 | -5.49 | 9.14 | 7.53 | 16.94 | -4.51 | -3.77 |
| 12 | n | n | -7.38 | -2.50 | -4.56 | -3.54 |
| 13 | -2.67 | -1.11 | -6.95 | -0.70 | -2.42 | -1.77 |
| 14 | -4.54 | -2.22 | -9.71 | -6.43 | -3.96 | -3.05 |
| 15 | 0.95 | -11.82 | -9.85 | -14.20 | 1.08 | 0.81 |
| 16 | -4.29 | -3.05 | n | n | n | n |
| 17 | -2.88 | 2.47 | -0.04 | -1.96 | -2.16 | -1.94 |
|   |     |     |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|-----|-----|
| 18| -6.12| 8.71| 10.51| 20.11| -5.06| -4.11|     |     |
| 19| n   | n   | n   | n   | n   | n   | n   |     |
| 20| n   | n   | 4.07| 12.09| 0.69 | 0.74|     |     |
| 21| -3.31| 10.08| -2.12| -4.58| -2.48| -2.39|     |     |
| 22| n   | n   | n   | n   | n   | n   |     |     |
| 23| -6.05| 4.78| -9.10| -3.83| -4.68| -3.95|     |     |
| 24| n   | n   | n   | n   | n   | n   |     |     |
| 25| -6.75| 3.69| -2.95| 2.55 | -5.68| -4.53|     |     |
| 26| n   | n   | n   | n   | n   | n   |     |     |
| 27| -6.00| 10.08| -8.22| -5.07| -4.91| -3.95|     |     |
| 28| -6.18| 8.65 | -1.50| 1.76 | -5.18| -4.04|     |     |
| 29| n   | n   | -7.18| -2.72| -4.91| -3.61|     |     |
| 30| -6.69| 7.75 | -8.71| -3.62| -5.19| -4.30|     |     |
| 31| n   | n   | n   | n   | n   | n   |     |     |
| 32| -6.61| 6.40 | -1.26| 3.47 | -5.43| -4.43|     |     |
| 33| -5.39| 1.56 | -8.26| -3.36| -4.77| -3.82|     |     |
| 34| n   | n   | -6.53| -4.36| -5.13| -4.18|     |     |
| 35| 3.79 | -1.83| 12.50| 13.49| 2.65 | 2.19|     |     |
| 36| -5.91| 7.18 | 13.88| 24.37| -4.55| -3.66|     |     |
| 37| n   | n   | n   | n   | n   | n   |     |     |
| 38| n   | n   | n   | n   | n   | n   |     |     |
| 39| 2.83 | -12.94| n   | n   | n   | n   |     |     |
| 40| 5.04 | -11.36| -1.94| -0.16| 3.60 | 2.94|     |     |
| 41| 8.88 | -6.15 | -7.87| -26.40| 7.08 | 5.75|     |     |
| 42| -1.42| 10.62 | -5.72| -11.61| -1.28| -1.05|     |     |
| 43| -2.21| 12.31| -7.68| -13.33| -1.97| -1.67|     |     |
| 44| -6.77| 11.48| -7.98| -4.37| -5.55| -4.51|     |     |
| 45| -6.40| 11.19| -4.24| 3.00 | -5.08| -3.97|     |     |
| 46| n   | n   | n   | n   | n   | n   |     |     |
| 47| n   | n   | -9.05| -4.39| -4.45| -3.53|     |     |
| 48| -2.37| 4.17 | 10.83| 22.97 | -2.24| -1.55|     |     |
| 49| -0.11| -2.09 | -3.50| 2.83 | -0.68| -0.37|     |     |
| 50| -5.65| 11.90| -5.86| -3.92| -4.88| -3.95|     |     |
| 51| -7.09| 2.16 | 6.79 | 15.69| -5.09| -4.06|     |     |
| 52| -0.32| 1.47 | 16.98| 27.26| -0.84| -0.76|     |     |
| 53| n   | n   | n   | n   | n   | n   |     |     |
| 54| 1.11 | 2.95 | 6.30 | 5.53 | 0.53 | 0.60|     |     |
| 55| -6.08| 2.00 | -6.76| -2.25| -4.81| -3.82|     |     |
| 56| 6.66 | -17.44| -11.02| -19.04| 5.25 | 3.95|     |     |
| 57| 9.67 | -18.22| n   | n   | n   | n   |     |     |
| 58| -0.61| -10.03| -7.86| -12.08| 0.07 | -0.28|     |     |
| 59| 2.50 | -13.04| -10.40| -12.03| 2.52 | 1.61|     |     |
| 60| 8.17 | -3.77 | -7.36| -25.03| 6.38 | 5.13|     |     |
| 61| 2.17 | 2.92 | -6.91| -19.07| 1.77 | 1.18|     |     |
| 62| 10.44| -12.75| -2.51| -16.25| 8.05 | 6.51|     |     |
| 63| -1.53| 2.99 | 11.05| 15.43| -1.44| -1.09|     |     |
|   | A23 | A24 | A25 | A26 | A27 | A28 |
|---|-----|-----|-----|-----|-----|-----|
| 64 | 5.26 | -13.70 | -10.72 | -22.60 | 4.48 | 3.27 |
| 65 | 8.40 | -5.75 | -4.03 | -19.75 | 6.08 | 5.07 |
| 66 | 2.06 | -12.83 | -11.32 | -16.22 | 1.37 | 1.09 |
| 67 | 0.82 | -8.28 | -9.85 | -8.13 | 0.24 | 0.31 |
| 68 | -6.32 | 9.33 | -8.74 | -4.57 | -5.39 | -4.60 |
| 69 | n   | n   | n   | n   | n   | n   |
| 70 | 1.01 | 7.41 | -4.55 | -13.50 | 0.78 | 0.43 |
| 71 | 6.10 | 0.33 | -6.23 | -21.30 | 4.82 | 3.74 |
| 72 | 10.12 | -13.75 | n   | n   | n   | n   |
| 73 | -5.07 | 14.45 | n   | n   | n   | n   |
| 74 | n   | n   | -5.46 | -6.60 | 0.19 | -0.30 |
| 75 | n   | n   | n   | n   | n   | n   |
| 76 | 0.16 | -0.88 | -1.12 | -1.70 | 0.02 | -0.02 |

**A23-A28:**

| Pub | A23 | A24 | A25 | A26 | A27 | A28 |
|-----|-----|-----|-----|-----|-----|-----|
| Source | T2001 | T2001 | T2001 | T2001 | T2001 | T2001 |
| Identify | DIDC5 | DIDC6 | DIDC7 | DIDC8 | DIDC9 | DIDC10 |
| D23M | x   | x   | x   | x   | x   | x   |
| 1   | n   | n   | n   | n   | n   | n   |
| 2   | -3.35 | -2.85 | -3.81 | -3.47 | 4.05 | 1.58 |
| 3   | -0.75 | -0.44 | -0.41 | -0.54 | -5.65 | -1.52 |
| 4   | -1.21 | -0.95 | -0.37 | -1.21 | -0.80 | -0.33 |
| 5   | -1.16 | -0.91 | -0.07 | -1.44 | 4.68 | 1.17 |
| 6   | -3.39 | -2.87 | -2.81 | -3.93 | 6.78 | 3.42 |
| 7   | -3.18 | -2.71 | -2.69 | -3.71 | 9.70 | 4.38 |
| 8   | -0.11 | -0.02 | -0.67 | 0.22 | -7.58 | 0.27 |
| 9   | n   | n   | n   | n   | n   | n   |
| 10  | n   | n   | n   | n   | n   | n   |
| 11  | -3.13 | -2.67 | -3.41 | -3.43 | 9.15 | 2.70 |
| 12  | -2.82 | -2.61 | -2.38 | -3.19 | 7.34 | 4.06 |
| 13  | -1.50 | -1.30 | -0.42 | -1.98 | 7.15 | 1.76 |
| 14  | -2.51 | -2.16 | -1.75 | -3.07 | 3.09 | 1.66 |
| 15  | 0.62 | 0.47 | 0.94 | 0.75 | -7.42 | -2.50 |
| 16  | n   | n   | n   | n   | n   | n   |
| 17  | -1.68 | -1.49 | -2.11 | -1.62 | -4.70 | 0.18 |
| 18  | -3.27 | -2.80 | -3.65 | -3.47 | 7.93 | 2.38 |
| 19  | n   | n   | n   | n   | n   | n   |
| 20  | 0.58 | 0.59 | 1.22 | 0.64 | 8.28 | -0.55 |
| 21  | -2.27 | -1.88 | -2.35 | -2.18 | -2.36 | 2.42 |
| 22  | n   | n   | n   | n   | n   | n   |
| 23  | -3.13 | -2.75 | -2.32 | -3.45 | 7.20 | 3.78 |
|   | n | n | n | n | n | n | n |
|---|---|---|---|---|---|---|---|
| 24 | n | n | n | n | n | n | n |
| 25 | -3.80 | -3.29 | -3.61 | -4.24 | 5.87 | 2.93 |
| 26 | n | n | n | n | n | n | n |
| 27 | -3.39 | -2.96 | -2.95 | -3.69 | 6.73 | 4.83 |
| 28 | -3.48 | -2.79 | -3.32 | -3.84 | 5.00 | 3.46 |
| 29 | -3.24 | -2.76 | -2.52 | -3.51 | 4.69 | 2.44 |
| 30 | -3.58 | -3.11 | -2.88 | -3.95 | 7.53 | 4.30 |
| 31 | n | n | n | n | n | n | n |
| 32 | -3.59 | -3.12 | -3.67 | -4.25 | 6.14 | 3.31 |
| 33 | -3.21 | -2.70 | -2.31 | -3.44 | 5.59 | 2.79 |
| 34 | -3.33 | -2.85 | -3.04 | -3.76 | 5.15 | 4.14 |
| 35 | 1.84 | 1.61 | 1.21 | 2.05 | 1.83 | -2.16 |
| 36 | -3.21 | -2.69 | -3.77 | -3.43 | 8.52 | 1.76 |
| 37 | n | n | n | n | n | n | n |
| 38 | n | n | n | n | n | n | n |
| 39 | n | n | n | n | n | n | n |
| 40 | 2.56 | 2.21 | 3.48 | 2.75 | 1.76 | -2.82 |
| 41 | 4.49 | 3.69 | 4.06 | 5.52 | -17.30 | -4.02 |
| 42 | -1.03 | -0.90 | -1.64 | -1.17 | -2.24 | 2.67 |
| 43 | -1.52 | -1.32 | -1.81 | -1.57 | -2.24 | 3.15 |
| 44 | -3.76 | -3.11 | -3.38 | -4.50 | 6.94 | 4.91 |
| 45 | -3.13 | -2.60 | -2.60 | -3.72 | 10.03 | 4.77 |
| 46 | n | n | n | n | n | n | n |
| 47 | -2.85 | -2.28 | -2.24 | -3.30 | 6.52 | 3.68 |
| 48 | -1.21 | -0.99 | -1.06 | -1.56 | 12.71 | 1.43 |
| 49 | -0.26 | -0.11 | 0.63 | -0.33 | 7.64 | 0.65 |
| 50 | -3.15 | -2.73 | -2.84 | -3.73 | 5.27 | 4.35 |
| 51 | -3.49 | -3.09 | -3.77 | -3.92 | 6.05 | 1.44 |
| 52 | -0.60 | -0.76 | 0.91 | 0.69 | 9.71 | -0.60 |
| 53 | n | n | n | n | n | n | n |
| 54 | 0.30 | 0.22 | -0.07 | 0.41 | 0.98 | -0.03 |
| 55 | -3.21 | -2.75 | -2.63 | -3.48 | 4.86 | 2.40 |
| 56 | 3.43 | 3.47 | 4.02 | 3.85 | -9.93 | -4.73 |
| 57 | n | n | n | n | n | n | n |
| 58 | 0.03 | -0.22 | -0.03 | -0.11 | -7.84 | -2.12 |
| 59 | 1.43 | 1.26 | 2.31 | 1.69 | -2.72 | -2.33 |
| 60 | 4.15 | 3.42 | 3.51 | 4.69 | -16.23 | -3.26 |
| 61 | 0.85 | 0.72 | 0.20 | 1.25 | -12.29 | -0.70 |
| 62 | 5.32 | 4.51 | 5.18 | 5.87 | -13.58 | -5.74 |
| 63 | -0.81 | -0.93 | -1.45 | -1.15 | 5.06 | 0.33 |
| 64 | 2.68 | 2.34 | 2.58 | 3.18 | -14.99 | -4.22 |
| 65 | 4.24 | 3.46 | 3.93 | 4.73 | -13.81 | -3.89 |
| 66 | 0.98 | 0.88 | 1.57 | 1.18 | -7.39 | -2.55 |
| 67 | 0.31 | 0.33 | 1.39 | 0.27 | 1.96 | -0.69 |
| 68 | -3.70 | -3.01 | -3.00 | -4.32 | 7.30 | 4.65 |
| 69 | n | n | n | n | n | n | n |
|   | A29 | A30 | A31 | A32 | A33 | A34 |
|---|-----|-----|-----|-----|-----|-----|
| pub | A29 | A30 | A31 | A32 | A33 | A34 |
| source | T2001 | R2005 | R2005 | R2005 | R2005 | R2005 |
| identify | DIDC11 | R1 | R2 | R3 | R4 | R5 |
| D23M | x | x | x | x | x | x |
| 1 | n | n | n | n | n | n |
| 2 | 11.40 | 10.13 | 13.01 | 10.31 | 9.09 | 7.41 |
| 3 | -3.66 | -12.11 | -15.41 | -10.51 | -7.79 | -7.70 |
| 4 | -4.23 | n | n | -10.11 | -8.11 | -6.75 |
| 5 | -1.70 | -2.43 | -1.34 | -3.41 | -3.63 | -1.68 |
| 6 | -2.05 | 5.43 | 14.09 | 4.70 | 3.08 | 4.58 |
| 7 | 5.36 | 15.00 | 23.41 | 12.83 | 8.65 | 9.34 |
| 8 | -2.48 | 0.53 | 2.74 | -0.81 | 0.41 | -2.18 |
| 9 | n | n | n | n | n | n |
| 10 | n | n | n | n | n | n |
| 11 | 12.31 | 15.19 | 19.05 | 14.30 | 10.92 | 10.63 |
| 12 | 1.02 | 11.51 | 22.09 | 10.63 | 6.38 | 8.40 |
| 13 | 1.55 | 1.49 | 3.75 | 0.19 | -0.83 | 0.56 |
| 14 | -3.15 | -1.02 | 1.27 | -2.49 | -2.34 | -0.57 |
| 15 | -5.42 | n | n | n | n | n |
| 16 | n | n | n | n | n | n |
| 17 | 3.94 | 1.82 | 3.81 | 2.83 | 2.28 | n |
| 18 | 14.25 | 14.52 | n | 14.79 | 11.90 | 10.83 |
| 19 | n | n | n | n | n | n |
| 20 | 7.25 | -1.82 | -4.70 | -1.17 | -1.37 | -0.51 |
| 21 | 3.53 | 12.16 | 18.04 | 10.79 | 7.88 | 5.78 |
| 22 | n | n | n | n | n | n |
| 23 | -2.14 | 8.76 | n | n | n | 4.24 |
| 24 | n | n | n | n | n | n |
| 25 | -1.81 | 8.35 | 13.30 | 6.28 | 4.65 | 6.60 |
| 26 | n | n | n | n | n | n |
| 27 | -2.88 | n | n | 11.33 | 8.08 | 8.85 |
| 28 | -3.36 | 14.20 | n | n | n | n |
| 29 | -2.89 | 3.78 | 6.72 | 1.92 | 1.56 | 3.11 |
| 30 | -1.84 | 11.00 | 19.97 | 7.96 | 5.45 | 6.48 |
| 31 | n     | n     | n     | n    | n    | n    |
| 32 | -2.43 | 11.16 | 18.63 | 9.12 | 7.32 | 8.77 |
| 33 | -2.47 | 4.05  | 8.69  | 2.35 | 1.14 | 3.09 |
| 34 | -4.52 | 13.23 | 21.78 | 10.37| 7.37 | 8.63 |
| 35 | 0.10  | -1.52 | -5.27 | -0.19| 1.17 | 1.63 |
| 36 | 13.82 | 13.40 | 16.11 | 13.84| 11.01| 11.19|
| 37 | n     | n     | n     | n    | n    | n    |
| 38 | n     | n     | n     | n    | n    | n    |
| 39 | n     | n     | n     | n    | n    | n    |
| 40 | 0.31  | n     | n     | -11.85| -9.56| -8.41|
| 41 | -13.87| -15.57| -21.38| -14.70| -10.77| -13.36|
| 42 | -8.05 | n     | n     | n    | 5.41 | n    |
| 43 | -5.91 | n     | n     | n    | 7.41 | 6.72 |
| 44 | -2.30 | 13.79 | 19.53 | 10.39| 7.72 | 9.12 |
| 45 | 4.97  | n     | n     | n    | n    | 10.45|
| 46 | n     | n     | n     | n    | n    | n    |
| 47 | -2.26 | 8.99  | 15.34 | 6.59 | 4.08 | 5.93 |
| 48 | 13.61 | 10.12 | n     | 9.74 | 7.67 | 8.05 |
| 49 | 3.70  | -0.94 | -0.52 | -1.65| -1.88| -0.06|
| 50 | -4.37 | n     | n     | 7.33 | 6.64 | 7.45 |
| 51 | 5.80  | 6.66  | n     | 7.04 | 6.52 | 7.08 |
| 52 | 10.64 | 5.46  | 4.21  | 6.27 | 6.64 | 5.70 |
| 53 | n     | n     | n     | n    | n    | n    |
| 54 | -3.68 | 4.43  | 5.40  | 4.51 | 3.97 | 4.80 |
| 55 | -3.17 | n     | n     | 2.80 | 1.71 | 3.19 |
| 56 | -8.47 | n     | n     | n    | -16.96| -15.48|
| 57 | n     | n     | n     | n    | n    | n    |
| 58 | -3.99 | -14.21| n     | -13.55| -9.93| -9.69|
| 59 | -5.08 | n     | -34.84| -16.14| n    | -11.90|
| 60 | -13.71| -12.46| -15.93| -11.08| -8.89| -10.98|
| 61 | -5.55 | -1.72 | -0.39 | -1.85| -1.70| -4.47|
| 62 | -10.95| -20.60| -29.04| -19.04| -13.98| -14.71|
| 63 | 1.34  | 6.71  | 7.48  | 6.91 | 6.47 | 6.89 |
| 64 | -8.78 | -20.86| -28.68| -20.99| -14.98| -18.25|
| 65 | -13.13| n     | n     | n    | n    | n    |
| 66 | -6.13 | -20.07| -25.83| -18.45| -14.16| -14.28|
| 67 | -2.62 | -10.54| -14.04| -9.61 | -8.82| -6.72 |
| 68 | -2.12 | 13.56 | 20.54 | 9.44 | 6.99 | 7.46 |
| 69 | n     | 16.26 | n     | 13.51| 9.85 | n    |
| 70 | -9.89 | 6.33  | 10.67 | 3.91 | 3.32 | 2.14 |
| 71 | -12.16| n     | n     | -7.05| -6.48| -7.43|
| 72 | n     | n     | n     | n    | n    | n    |
| 73 | n     | -12.26| -16.54| -11.37| -9.09| -9.05 |
| 74 | -4.31 | -6.96 | -9.02 | -6.73| -4.85| -4.46|
| 75 | n     | n     | n     | n    | n    | n    |
| pub | A35 | A36 |
|-----|-----|-----|
| source | R2005 | R2005 |
| identify | R6 | R7 |
| D23M | x | x |
| 1 | n | n |
| 2 | 8.44 | 1.58 |
| 3 | -5.87 | -1.52 |
| 4 | -6.77 | -0.33 |
| 5 | -4.79 | 1.17 |
| 6 | -3.01 | 3.42 |
| 7 | 1.86 | 4.38 |
| 8 | -3.46 | 0.27 |
| 9 | n | n |
| 10 | n | n |
| 11 | 8.88 | 2.70 |
| 12 | -1.41 | 4.06 |
| 13 | -2.42 | 1.76 |
| 14 | -4.77 | 1.66 |
| 15 | -7.76 | -2.50 |
| 16 | n | -0.38 |
| 17 | 1.62 | 0.18 |
| 18 | 11.01 | 2.38 |
| 19 | n | n |
| 20 | 2.93 | -0.55 |
| 21 | 1.95 | 2.42 |
| 22 | n | n |
| 23 | -2.71 | 3.78 |
| 24 | n | 4.22 |
| 25 | 0.08 | 2.93 |
| 26 | n | 3.22 |
| 27 | -1.41 | 4.83 |
| 28 | 1.13 | 3.46 |
| 29 | -2.60 | 2.44 |
| 30 | -1.96 | 4.30 |
| 31 | n | n |
| 32 | 1.24 | 3.31 |
| 33 | -3.12 | 2.79 |
| 34 | -1.52 | 4.14 |
| 35 | 5.33 | -2.16 |
| 36 | 11.76 | 1.76 |
| 37 | n | n |
|   |   |   |
|---|---|---|
| 38 | n | n |
| 39 | n | -2.88 |
| 40 | -3.15 | -2.82 |
| 41 | -9.26 | -4.02 |
| 42 | -2.40 | 2.67 |
| 43 | -2.50 | 3.15 |
| 44 | -1.28 | 4.91 |
| 45 | 1.94 | 4.76 |
| 46 | n | n |
| 47 | -3.06 | 3.68 |
| 48 | 9.35 | 1.43 |
| 49 | -0.99 | 0.65 |
| 50 | -0.38 | 4.35 |
| 51 | 6.33 | 1.44 |
| 52 | 11.11 | -0.60 |
| 53 | n | n |
| 54 | 3.22 | -0.03 |
| 55 | -2.85 | 2.40 |
| 56 | -11.01 | -4.73 |
| 57 | n | -6.35 |
| 58 | -6.10 | -2.12 |
| 59 | -8.51 | -2.33 |
| 60 | -8.55 | -3.26 |
| 61 | -4.68 | -0.70 |
| 62 | -7.22 | -5.74 |
| 63 | 6.97 | 0.33 |
| 64 | -10.20 | -4.22 |
| 65 | -5.57 | -3.88 |
| 66 | -9.30 | -2.55 |
| 67 | -6.51 | -0.69 |
| 68 | -1.76 | 4.65 |
| 69 | -0.20 | 4.63 |
| 70 | -3.44 | 1.11 |
| 71 | -7.02 | -2.18 |
| 72 | n | n |
| 73 | -6.33 | -2.37 |
| 74 | -3.27 | -0.17 |
| 75 | n | n |
| 76 | -0.95 | -0.23 |

n = no data available

Table S6:
For NH rdc data sets taken from the literature, the following nomenclature has been used:

| Name | Alignment conditions | Reference | Ref. Abbreviation |
|------|----------------------|-----------|------------------|
| A14  | E1                   | Lakomek et al., 2006 | L2006 |
| A15  | E2                   | Lakomek et al., 2006 | L2006 |
| A16  | E3                   | Lakomek et al., 2006 | L2006 |
| A17  | E4                   | Lakomek et al., 2006 | L2006 |
| A18  | E5                   | Lakomek et al., 2006 | L2006 |
| A19  | Bic1                 | Ottiger and Bax, 1998 | O1998 |
| A20  | Bic2                 | Ottiger and Bax, 1998 | O1998 |
| A21  | PM1                  | Briggman and Tolman, 2003 | B2003 |
| A22  | PM2                  | Briggman and Tolman, 2003 | B2003 |
| A23  | PM3                  | Briggman and Tolman, 2003 | B2003 |
| A24  | PM4                  | Briggman and Tolman, 2003 | B2003 |
| A25  | PM5                  | Briggman and Tolman, 2003 | B2003 |
| A26  | PM6                  | Briggman and Tolman, 2003 | B2003 |
| A27  | Helfrich             | Briggman and Tolman, 2003 | B2003 |
| A28  | Phage                | Briggman and Tolman, 2003 | B2003 |
| A29  | C12E5                | Briggman and Tolman, 2003 | B2003 |
| A30  | A                    | Ruan and Tolman, 2005 | R2005 |
| A31  | B                    | Ruan and Tolman, 2005 | R2005 |
| A32  | C                    | Ruan and Tolman, 2005 | R2005 |
| A33  | D                    | Ruan and Tolman, 2005 | R2005 |
| A34  | E                    | Ruan and Tolman, 2005 | R2005 |
| A35  | F                    | Ruan and Tolman, 2005 | R2005 |
| A36  | G                    | Ruan and Tolman, 2005 | R2005 |

Note:

For convenience, all NH rdc data sets used for the SCRM analysis are provided in Table S5, including data sets taken from the Supporting Information by Tolman and coworkers, with permission by J. Tolman. Please note the references to the original literature.

The NH rdc data sets A19 to A29 are those provided in the supplement to (Brigmann and Tolman, 2003). Data sets A30 to A36 have been taken from the Supporting Information to (Ruan and Tolman, 2005). Data sets taken from the literature are referenced in the same way as in the original literature. We refer to the original literature for further information.
Figures

Figure S1:
Distribution function $F_{\text{max}}(b)$

Figure S2:
a) and b): The difference of the inter-nuclear vector angle $\Delta(\theta_{av})$ between two SCRM cycles is plotted. After 4 cycles of SCRM the inter-nuclear vector angle $\theta_{av}$ deviate less than 0.5 degree between succeeding SCRM cycles for a) D23M and b) D36M, the same holds for difference of the inter-nuclear vector angle $\Delta(\phi_{av} \cdot \sin \theta_{av})$. The inter-nuclear vector orientation $(\phi_{av}, \theta_{av})$ converges to a dynamic average that fulfils the NH RDC data best.

c) and d): The inter-nuclear angles $\kappa_j$ enclosed between the dynamic average NH vector orientations derived from c) D23M and d) D36M using the 1d3z NMR structure as starting structure and the NH vectors of the starting 1d3z NMR structure itself are shown. The average angular deviation is 4.76° for D23M and 4.71° for D36M.
e) The inter-nuclear angle $\kappa_j$ enclosed between the dynamic average vectors derived from D23M and derived from D36M agree very well with and average $\kappa$ value of 1.4° (compare Supporting Information Figure S2e). A higher deviation is observed for Gly35 and Asp52 which also show a higher discrepancy of the $S_{rdc}^2$.

Literature

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Figure S1
Figure S2