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 6^{th} and higher singular values to differ from zero. The ratio of the 5^{th} and 6^{th} 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 5^{th} 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

$$\mathbf{C} = \mathbf{B}^T\mathbf{B}$$

where $\mathbf{B} = (\mathbf{e}_1, \mathbf{e}_2, \ldots \mathbf{e}_N)$ is the 3xN matrix containing the normalized NH vectors $\mathbf{e}_k$ 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 rdcs of D23M

The RDCs D_{MF} 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 ± 0.5. We found that Gaussian noise of σ = 0.22 Hz on the RDCs back-calculated for D23M led to this SECONDA gap of 6.5 ± 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^2_{rdc}

The following order parameters S^2_{rdc} are obtained using the experimental NH RDC data collection D23M. The first line is the residue number, second line the order parameter S^2_{rdc}, third the error on the S^2_{rdc} values propagated from the experimental error $\sigma_j^{\exp}$ = 0.3 Hz and fourth line the error on the S^2_{rdc} 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:

D23M

#	S^2_{rdc}	*Exp. Err.*	*Exp. +Me. Err.*
1	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
10	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
17	0.86	0.06	0.06
18	0.77	0.04	0.04
19	n	n	n
20	0.55	0.05	0.05
21	0.86	0.05	0.05
22	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

71	0.57	0.03	0.04
72	n	n	n
73	n	n	n
74	0.17	0.02	0.04
75	n	n	n
76	0.02	0.01	0.01

n= no data available

Table S2:

D36M

#	S^2_{rdc}	*Exp. Err.*	*Exp. +Me. Err.*
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
26	0.78	0.06	0.08
27	0.82	0.04	0.04
28	0.82	0.04	0.09
29	0.78	0.04	0.05
30	0.79	0.03	0.04
31	n	n	n
32	0.85	0.04	0.04
33	0.75	0.03	0.04
34	0.75	0.03	0.04
35	0.64	0.03	0.08
36	0.77	0.04	0.08
37	n	n	n
38	n	n	n
39	0.68	0.03	0.07
40	0.71	0.03	0.08
41	0.77	0.02	0.04
42	0.74	0.03	0.03
43	0.75	0.03	0.08
44	0.75	0.03	0.09
45	0.78	0.04	0.07
46	n	n	n
47	0.79	0.05	0.05
48	0.58	0.02	0.06
49	0.77	0.04	0.08
50	0.63	0.03	0.10
51	0.84	0.05	0.08
52	0.62	0.01	0.03

53	n	n	n
54	0.64	0.03	0.08
55	0.77	0.04	0.04
56	0.76	0.02	0.04
57	0.86	0.02	0.04
58	0.84	0.05	0.09
59	0.83	0.03	0.03
60	0.80	0.02	0.04
61	0.83	0.03	0.03
62	0.57	0.01	0.03
63	0.68	0.03	0.05
64	0.79	0.04	0.07
65	0.63	0.02	0.05
66	0.81	0.03	0.06
67	0.83	0.03	0.04
68	0.83	0.03	0.05
69	n	n	n
70	0.72	0.03	0.03
71	0.67	0.02	0.04
72	0.56	0.03	0.05
73	n	n	n
74	0.20	0.02	0.03
75	n	n	n
76	0.02	0.01	0.01

Deviation between dynamic average inter-nuclear vector orientations and X-ray and NMR starting structure

Table S3 (D23M):

The inter-nuclear angles κ_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 $S^2_{rdc}(NH)$ and κ_j are listed in column 2 and 6 (see also Figure S2e). In column 1 the derived κ_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 κ_j.

residue #	S^2_{rdc} (1ubi)	S^2_{rdc} (1d3z)	κ ubi/ubi	κ ubi/1d3z	κ 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

72	n	n	n	n	n

n= no data available

Table S4: Same as Table S3 but for D36M.

residue #	S^2_{rdc} (1ubi)	S^2_{rdc} (1d3z)	κ ubi/ubi	κ ubi/1d3z	κ 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

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 $S^2_{overall}$

The scaling of the unscaled RDC-based $S^2_{rdc,unscaled}$ order parameters based on the Lipari-Szabo order parameter S^2_{LS} becomes non-trivial when taking the experimental error σ 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 $S^2_{overall}$ such that a confidence level $1-\alpha$ can be provided for the estimated $S^2_{overall}$.

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

$$\lambda^* = \underset{\lambda}{Max}\left\{\lambda f_i \le g_i\right\} = \underset{i=1,\ldots,n}{Min}\left\{\frac{g_i}{f_i}\right\} = \frac{1}{\underset{i=1,\ldots,n}{Max}\left\{\frac{f_i}{g_i}\right\}} = \frac{1}{\underset{i=1,\ldots,n}{Max}\left\{f_i^*\right\}}$$

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

σ_i^2 on the derived order parameters $S^2_{rdc,unscaled,i}$ that will be called Y_i in the following.

Because the true overall scaling factor λ^* is unknown, it will be estimated by

$$\hat{\lambda} = \frac{1}{\underset{i=1,\ldots,n}{Max}\left\{Y_i^*\right\}} \quad \text{with } Y_i^* = \frac{Y_i}{g_i} .$$

Now we want to give an upper bound for the true λ^* 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 λ^*: $P\left(\lambda^* < \hat{\lambda}_\alpha^u\right) = 1-\alpha$? 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

$F_{\max}(b) = P\left(\underset{i}{Max}\, Y_i^* - \underset{i}{Max} f_i^* \le b\right)$ 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, $F_{\max}(b)$ 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 σ_i^2 around the unknown true order parameter $Y_i = f_i + \varepsilon(\sigma_i)$ (where the error $\varepsilon(\sigma_i)$ 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 σ_i^2. Accordingly, we have generated new data with expectation of our experimental vector $Y^* = EY_j$.

The distribution function is constructed out of the N different Y_j^* curves. We calculate N times $\underset{i}{Max}\, Y_{ij}^* - \underset{i}{Max} f_i^*$ for the different Y_j^* and by this generate the distribution function $F_{\max}(b)$ (compare Figure S1).

Starting from $1-\alpha = F_{\max}(b) = P\left(\underset{i}{Max}\, Y_i^* - \underset{i}{Max} f_i^* \le b \right)$ we can invert for the upper bound b. Using the relationship $\lambda^* = \dfrac{1}{\underset{i=1,\ldots,n}{Max}\left\{ f_i^* \right\}}$ gives

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

which can be transformed into

$$1-\alpha = P\left(\lambda^* \le \frac{1}{\dfrac{1}{\hat{\lambda}} - b} \right) = P\left(\lambda^* \le \hat{\lambda}_\alpha^u \right).$$

Now we obtain the required confidence bound $\hat{\lambda}_\alpha^u$ for the estimated scaling factor

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

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

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

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

$P\left(S_{overall} \le 0.89\right)$ = 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^2_{rdc} order parameters derived from D36M with respect to the Lipari-Szabo ones S^2_{LS}. 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 $\sigma_j^{rmsd} = rmsd(rdc, j)$, the confidence level is $P\left(S_{overall} \le 0.89\right)$=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^2_{LS} and S^2_{rdc} order parameters (at any scaling) might stem from the same distribution (zero supra-τ_c motion hypothesis). Practically, this is achieved by the generation of multiple sets of synthetic order parameters, gauss-distributed around the measured S^2_{rdc} order parameters with a standard deviation given by the respective uncertainties. The zero supra-τ_c motion hypothesis was rejected with a confidence of more than 99.999%, indicating significant supra-τ_c motion. To obtain a scaling estimate, the method successively removes residues that display the most significant supra-τ_c motion until the zero supra-τ_c 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^2_{LS} order

parameters is the suggested scaling factor. Uncertainties in order parameters were estimated both from the experimental error on the RDC's $\sigma_j^{\exp}$ = 0.3 Hz and from the average $\sigma_j^{rmsd} = rmsd(rdc, j)$ (0.5 Hz), yielding scaling factors $S^2_{overall}$ of 0.88 and 0.91.

These results corroborate the presence of supra-τ_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:

A1-A8:

	A1	A2	A3	A4	A5	A6	A7	A8
source	SCRM	SCRM	SCRM	SCRM	SCRM	SCRM	SCRM	SCRM
Identifier	A1	A2	A3	A4	A5	A6	A7	A8
D23M		x		x				
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

49	-2.36	-4.10	6.65	5.36	-2.37	-3.38	3.08	-2.99
50	0.24	-0.58	n	-4.82	n	n	-5.45	3.35
51	-3.50	-7.08	-21.66	7.60	5.29	3.86	10.97	7.13
52	-5.56	-12.26	-4.39	15.47	n	-0.20	24.86	7.78
53	n	n	n	n	n	n	n	n
54	-1.22	-4.31	0.90	-4.29	6.52	5.37	4.10	5.92
55	-1.72	-3.08	-13.20	-4.59	8.05	5.68	-5.64	1.51
56	4.72	8.68	n	-10.68	n	-30.37	-14.70	-6.92
57	6.61	13.21	33.68	-15.27	-39.89	-32.08	-20.14	-8.80
58	3.23	6.65	3.99	-5.97	-19.49	-15.67	-11.02	-4.39
59	1.32	3.11	18.26	-6.63	-24.78	-21.47	-10.57	-6.45
60	6.79	13.70	20.63	-18.09	-11.07	-7.34	-20.16	-6.09
61	6.24	12.98	2.02	-8.01	2.35	4.16	-15.78	-6.12
62	n	7.78	29.60	-14.32	-28.53	n	-11.07	-5.51
63	-3.53	-8.73	-9.76	2.42	6.92	4.91	13.06	7.97
64	6.39	13.42	21.55	-12.09	-30.39	-22.99	-18.96	-7.80
65	3.84	10.02	23.22	-17.50	-15.20	-11.38	-15.67	-5.31
66	3.12	6.91	14.14	-8.69	-26.04	-20.96	-14.92	-5.95
67	-0.28	0.36	4.63	-3.31	-14.65	-12.85	-7.64	-5.29
68	-1.58	-2.37	-17.91	-3.29	23.62	18.08	-7.53	-0.40
69	1.69	n	-15.96	-8.04	n	n	-11.95	-5.83
70	2.69	4.87	-1.26	-13.37	14.68	12.02	-12.89	-1.10
71	5.97	10.93	13.76	-16.17	-2.38	-0.87	-17.62	-5.35
72	3.14	5.91	n	-9.56	-30.26	-24.97	-7.62	-4.92
73	0.72	2.24	15.22	-1.78	n	n	-7.77	-1.48
74	n	n	3.37	-5.71	-9.35	-7.36	-8.14	-3.68
75	n	n	n	n	n	n	n	n
76	0.26	0.51	1.60	-1.59	-1.86	-1.39	-2.21	0.22

A9-A16:

	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
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	7.69	7.58	16.24	14.35	19.19	16.90	6.04	7.47
12	-17.41	-6.26	n	-7.45	-4.25	n	n	n
13	-14.33	-5.37	-10.95	-6.08	-1.49	-3.59	5.07	0.31
14	-12.51	-8.20	-15.99	-11.49	-7.75	-7.55	1.94	-2.54
15	-17.59	-8.75	-17.91	-15.28	-16.32	-14.52	-4.97	-3.64
16	-1.09	-1.40	-2.42	-0.61	0.48	-0.09	-1.45	0.76
17	-8.94	-0.16	-0.38	-0.23	-2.64	1.74	-3.13	2.19
18	12.84	10.08	16.51	20.94	23.35	19.92	5.40	8.64
19	n	n	n	n	n	n	n	n
20	n	n	n	n	n	n	n	n
21	n	-2.32	-3.90	-3.71	-6.88	1.41	-1.71	1.72
22	-25.50	-10.87	-20.94	-21.77	-27.32	n	n	n
23	n	-7.70	-18.30	-9.07	-5.64	-3.92	4.72	-1.94
24	n	n	n	n	n	n	n	n
25	6.56	-2.24	-5.57	-2.90	2.72	1.30	3.29	-1.39
26	-13.73	-7.54	-13.32	-9.16	-4.93	n	n	n
27	-11.08	-7.02	-14.14	-9.18	-6.56	-2.33	4.08	-2.35
28	12.12	-1.47	-3.02	0.09	1.76	2.12	2.73	-1.86
29	-5.10	-6.60	-12.58	-6.78	-3.49	n	n	n
30	-13.58	-7.43	-14.05	-8.67	-5.38	-2.67	4.78	-1.60
31	n	-4.43	-7.66	-5.64	n	n	n	n
32	11.16	-1.09	-1.95	0.03	3.71	3.23	3.27	-1.29
33	-9.02	-7.18	-14.48	-7.98	-4.26	-4.13	3.70	-1.87
34	-6.08	-5.88	-11.01	-7.39	-6.12	n	n	n
35	n	11.13	23.80	18.51	16.77	9.93	0.83	1.04
36	24.65	13.24	22.17	21.07	28.89	22.30	5.44	8.57
37	n	n	n	n	n	n	n	n
38	n	n	n	n	n	n	n	n
39	-20.05	-10.23	-19.32	-20.36	n	-17.22	-6.20	-4.55
40	-5.88	-0.88	-1.43	-1.95	0.83	-5.21	2.17	0.01
41	-19.92	-8.77	-18.92	-20.60	-30.17	-19.89	-11.62	-8.06
42	n	-5.35	-9.81	-9.94	-13.59	-5.72	-1.85	-4.70
43	-20.76	-7.89	-11.09	-13.24	-16.21	-6.00	-1.74	-3.42
44	-14.02	-7.02	-11.95	-8.72	-6.03	-2.16	4.27	-1.78
45	-16.37	-3.11	-4.72	-2.66	2.30	3.58	6.86	2.37
46	n	n	n	n	n	n	n	n
47	n	n	n	n	n	n	n	n
48	15.70	10.99	21.97	21.56	26.82	17.87	8.95	8.05
49	-11.67	-2.22	-4.88	-1.77	3.23	-1.18	5.68	1.55
50	-3.90	-4.26	-8.56	-4.80	-3.49	-0.54	3.45	-2.00
51	21.33	6.49	14.17	14.86	18.47	12.59	3.56	3.94
52	34.79	15.97	n	25.90	32.72	20.72	6.39	7.36
53	n	n	n	n	n	n	n	n
54	25.73	4.46	9.43	7.20	7.47	5.45	0.30	-1.18
55	-3.46	-5.72	-11.00	-7.27	-2.89	-3.70	2.99	-2.30
56	-21.59	-10.67	-19.82	-18.88	-21.02	-20.23	-5.54	-5.22

57	-25.52	-10.72	-22.87	-24.15	-29.51	-24.21	-10.68	-6.93
58	-12.86	-6.85	-15.35	-9.78	-13.84	-11.74	-5.65	-3.16
59	-20.54	-9.29	-17.61	-15.29	-14.63	-14.87	-1.22	-3.56
60	-16.60	-7.82	-12.97	-15.86	-28.26	-17.93	-10.82	-7.81
61	-24.88	-7.24	-13.06	-14.47	-22.72	-11.06	-8.16	-3.41
62	-3.96	-3.30	-4.37	-8.87	-18.15	-14.82	-8.81	-5.93
63	34.75	9.83	18.13	16.54	18.87	12.84	2.93	1.80
64	-24.42	-10.08	-20.04	-20.26	-26.67	-20.25	-9.47	-5.54
65	-6.47	-5.24	-8.33	-12.32	-22.35	-15.77	-9.80	-7.14
66	-20.72	-10.22	-18.45	-18.75	-18.75	-16.64	-4.65	-4.40
67	-18.86	-7.76	-16.14	-12.90	-9.13	-10.78	1.99	-2.37
68	-14.75	-7.85	-15.51	-10.19	-5.69	-3.19	4.79	-1.67
69	-16.20	-7.22	-13.69	-11.67	-13.66	n	n	n
70	-5.96	-5.25	-7.92	-9.66	-16.05	-7.87	-4.05	-5.53
71	-15.48	-6.69	-12.51	-16.39	-24.68	-15.40	-8.36	-6.95
72	-3.75	-3.12	-5.44	-8.81	-13.59	-13.51	-5.23	-4.89
73	-19.87	-5.97	-11.41	-7.74	-8.97	-1.19	1.90	n
74	-7.27	-4.52	-10.12	-8.12	-7.95	n	n	n
75	n	n	n	n	n	n	n	n
76	0.88	-1.16	-2.06	-2.41	-2.33	-1.64	-0.96	-0.65

A17-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
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

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

24	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
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
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
38	n	n	n	n	n	n
39	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
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
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
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

70	0.23	0.17	-0.07	0.39	-5.26	1.11
71	2.93	2.41	2.41	3.73	-12.31	-2.18
72	n	n	n	n	n	n
73	n	n	n	n	n	n
74	0.08	-0.10	0.11	-0.15	-2.28	-0.17
75	n	n	n	n	n	n
76	-0.02	-0.03	-0.09	n	-0.83	-0.23

A29-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
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	-2.13	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

76	-0.94	-1.56	-1.85	-1.50	-1.16	-1.14

A35-A36:

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 $F_{\max}(b)$

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 θ_{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 $\Delta(\phi_{av} \bullet \sin\theta_{av})$. The inter-nuclear vector orientation (ϕ_{av}, θ_{av}) converges to a dynamic average that fulfils the NH RDC data best.
c) and d): The inter-nuclear angles κ_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 κ_j enclosed between the dynamic average vectors derived from D23M and derived from D36M agree very well with and average κ 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^2_{rdc}.

Literature

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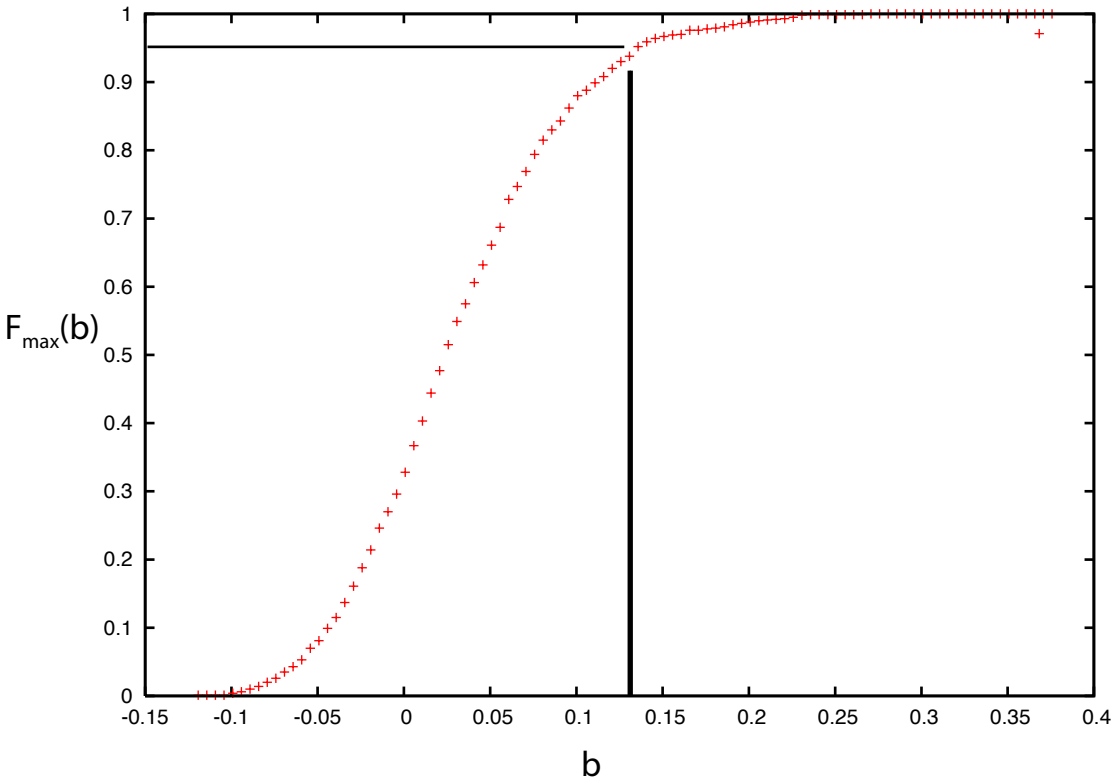
$F_{max}(b)$
b
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4

Figure S1

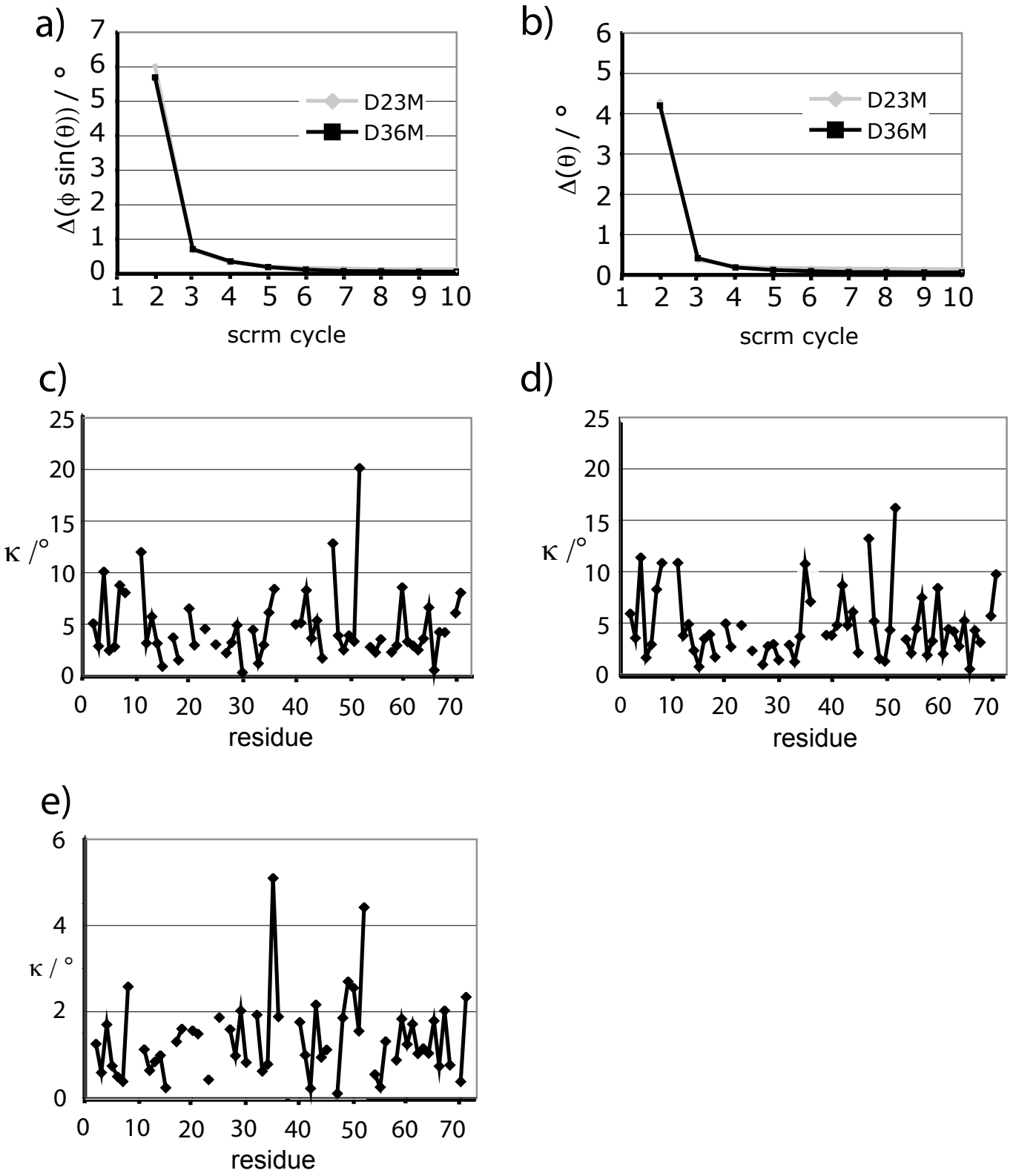
a)
Δ(ϕ sin(θ)) / °
D23M
D36M
scrm cycle
b)
Δ(θ) / °
D23M
D36M
scrm cycle
c)
κ /°
residue
d)
κ /°
residue
e)
κ / °
residue

Figure S2