Quantitative Conformational Analysis of Partially Folded Proteins from Residual Dipolar Couplings : Application to the Molecular Recognition Element of Sendai Virus Nucleoprotein

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Supporting Information

Figure S1

Helical propensity determined on the basis of $^{13}C_\alpha$ NMR secondary chemical shifts. The presence of secondary structure was estimated by subtracting random coil shifts.[1] Positive values indicate the presence of helical elements.

Figure S2

Propensity of different amino acids to be in the N-capping position in folded structures derived from a database of high resolution crystallographic structures (ref 47 in manuscript).

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[1] Wishart DS, Sykes BD (1994) The ^{13}C chemical-shift index: a simple method for the identification of protein secondary structure using ^{13}C chemical-shift data. *J. Biomol. NMR* 4 :171– 180.

Table S1 (Supporting Information)

Helical conformers[a] (population)[b]	χ^{2} [c]
476-487 (0.60)	662
478-489 (0.60)	653
479-487 (0.89)	621
476-488 (0.52)	427

Helical conformers[a] (population)[b]	χ^{2} [c]
476-484 (0.46) 479-488 (0.45)	265
476-488 (0.38) 479-492 (0.17)	259
476-488 (0.36) 488-492 (0.15)	253
476-488 (0.37) 479-484 (0.45)	227

Helical conformers[a] (population)[b]	χ^{2} [c]
476-488 (0.28) 479-484 (0.30) 478-483 (0.14)	138
476-488 (0.27) 479-484 (0.38) 478-493 (0.10)	131
476-488 (0.30) 479-484 (0.37) 478-495 (0.07)	124
476-488 (0.28) 479-484 (0.36) 478-492 (0.11)	121

Table S1 Data reproduction from ensembles with different numbers of helical conformers (top 4 data fits in each case)

a - Range of the invoked helices.

b - Population of the invoked helices. The remaining conformers are unfolded.

c - Target function measured over all 100 RDCs.

Figure S1

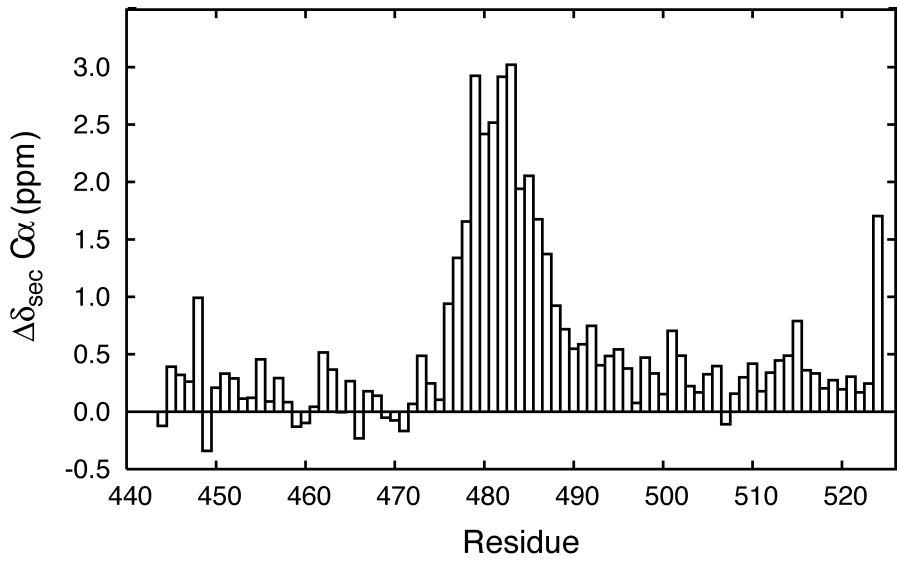
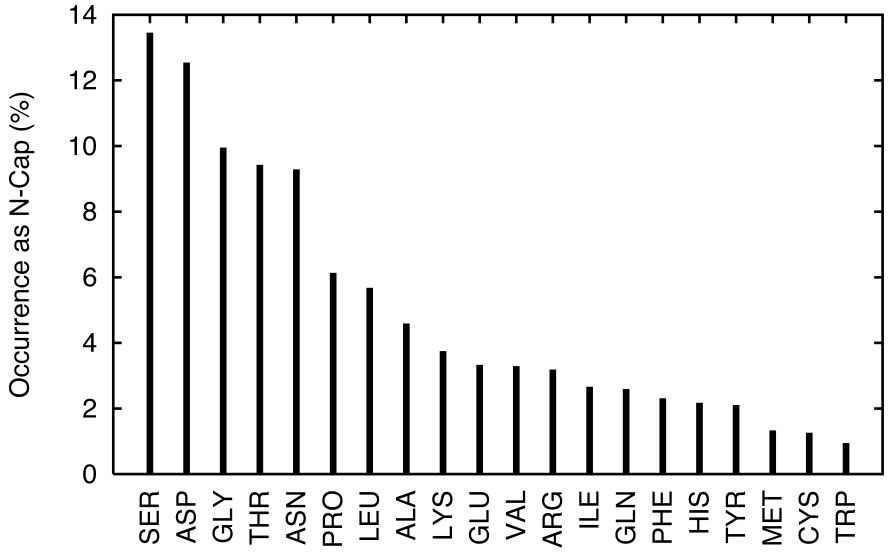

3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
440
450
460
470
480
490
500
510
520
Residue
Δδsec Cα (ppm)

Figure S2


Occurrence as N-Cap (%)
0
2
4
6
8
10
12
14
SER
ASP
GLY
THR
ASN
PRO
LEU
ALA
LYS
GLU
VAL
ARG
ILE
GLN
PHE
HIS
TYR
MET
CYS
TRP