BIOCHEMISTRY
including biophysical chemistry & molecular biology
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SUPPLEMENTARY MATERIAL

Figure 1. Strips from the following spectra of reduced uniformly $^{15}N/^{13}C$ labeled DsbA: CBCA(CO)NH (A), HNCA (B) and CBCANH (C). The arrangement shows the resonances of residues Asn156 - Asn162 belonging to the β-strands 4 and 5 of DsbA. The strips were taken at the ^{1}H and ^{15}N chemical shift of the residue of interest. The corresponding shifts are indicated below the strips. The ^{13}C-chemical shift is indicated at the right side of the figure. Black arrows mark the sequential connectivities between C^{α} atoms and white arrows mark the sequential connectivites between C^{β} atoms which can be derived from the three spectra.

Figure 2. A) Residue-based rms deviations of the backbone ϕ (red line) and ψ (green line) and side-chain χ1 (blue line) torsion angles from the averaged mean structure for the 20 SA structures.

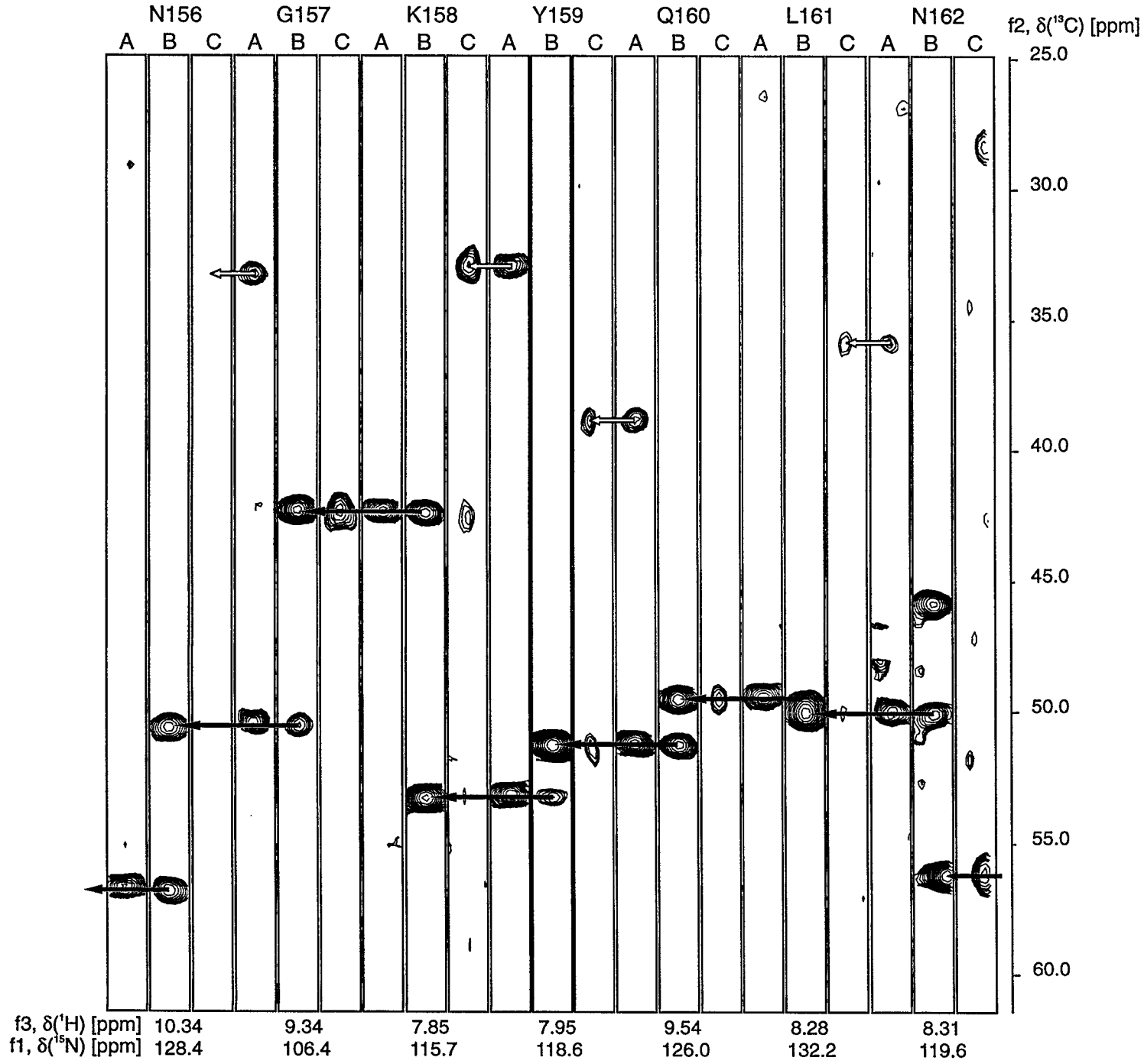
B) Plot of the number of NOE distance constraints per residue versus amino acid sequence of DsbA. All constraints appear twice, once for each interacting residue. No intra-residue constraints are shown. Sequential constraints are coloured red, medium range NOEs ($|i-j| < 5$) green, and long range NOEs ($|i-j| > 4$) are shown in blue.

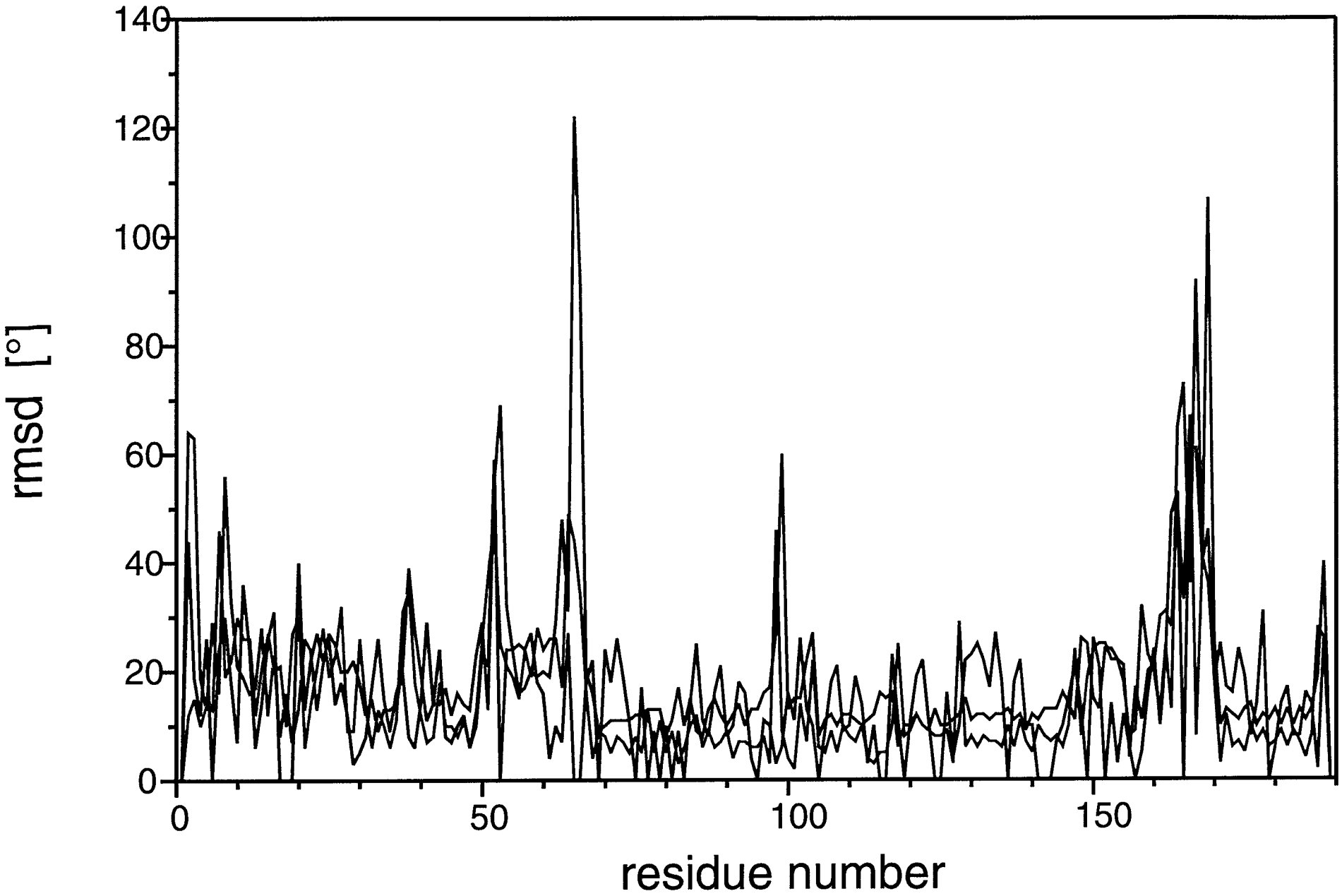
Figure 3. A) Ramachandran plot for the family of 20 SA structures of reduced DsbA. Glycine residues are indicated by blue crosses, all other residues by blue dots. The allowed regions were determined from 378 different crystal structures with

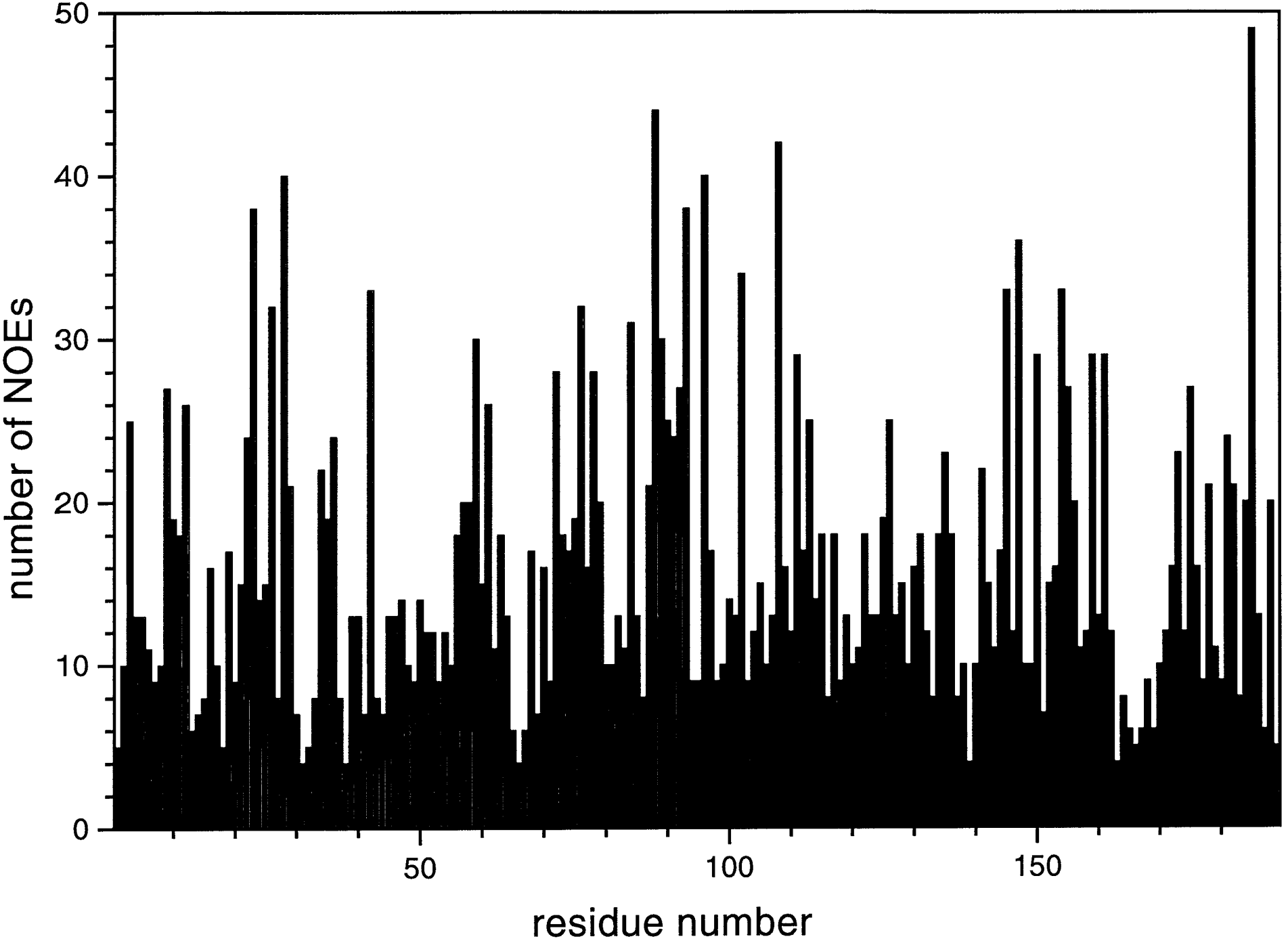
a resolution of 2.5 Å or better. The regions where the density of ϕ/ψ-points from this statistics is highest are marked in colour. The green regions contain 80% of all points, the green and yellow regions together 95% and all coloured regions together 98%. Figure produced with MOLMOL.

B) Ramachandran plot for the energy minimized average structure of reduced DsbA and for the crystal structure of oxidized DsbA. Glycine residues are indicated by crosses, all other residues by dots. The energy minimized average structure of reduced DsbA is indicated by blue symbols. Red and orange symbols represent molecule A and molecule B, respectively, from the crystal structure of oxidized DsbA. Figure produced with MOLMOL.

Figure 4. Sausage plot showing a smooth spline curve through the positions of the C^{α} atoms of the protein backbone. The diameter of the spline curve is proportional to the rmsd of the structure family from the mean structure. The N and C terminus of the protein are depicted. Figure produced with MOLMOL.


N156
G157
K158
Y159
Q160
L161
N162
A B C A B C A B C A B C A B C A B C A B C
f2, δ(13C) [ppm]
25.0
30.0
35.0
40.0
45.0
50.0
55.0
60.0
f3, δ(1H) [ppm] 10.34 9.34 7.85 7.95 9.54 8.28 8.31
f1, δ(15N) [ppm] 128.4 106.4 115.7 118.6 126.0 132.2 119.6


140
120
100
80
60
40
20
0
rmsd [°]
0
50
100
150
residue number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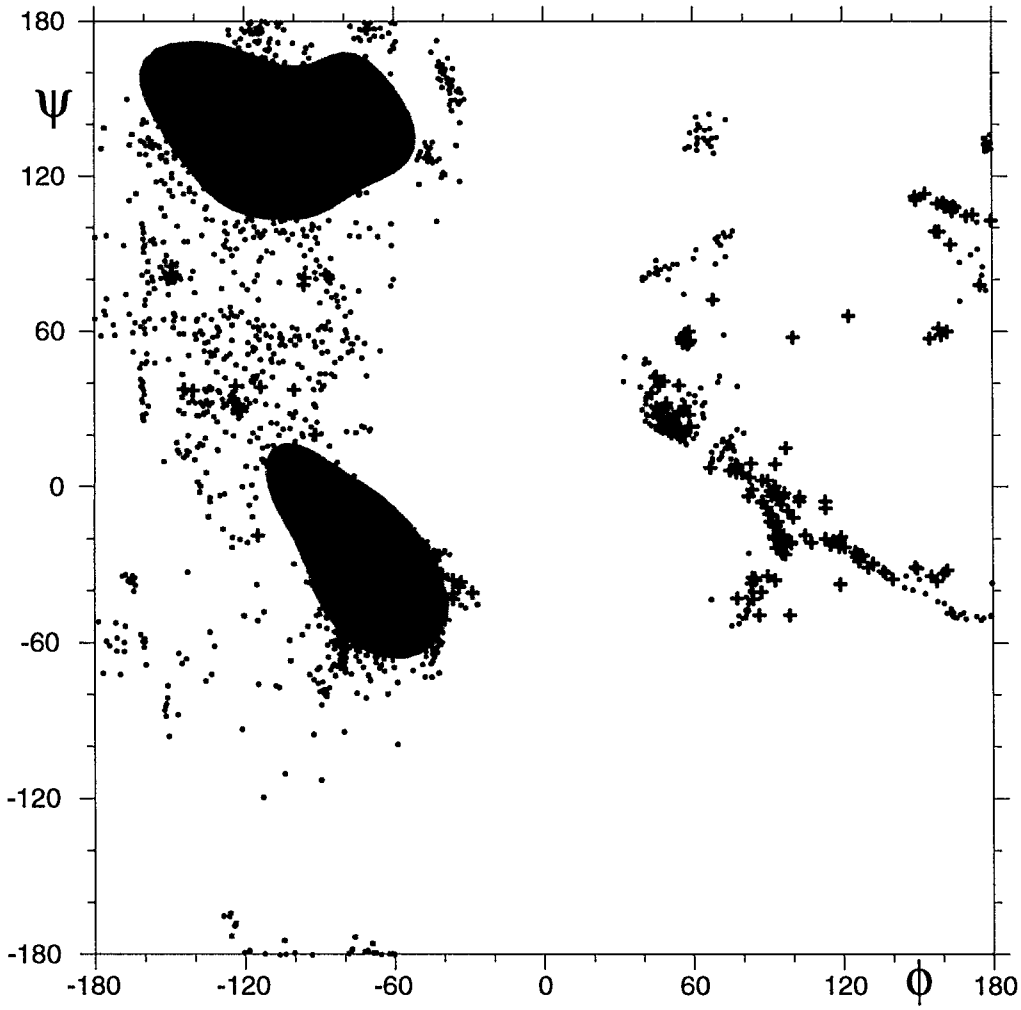
40
30
20
10
0
number of NOEs
50
100
150
residue number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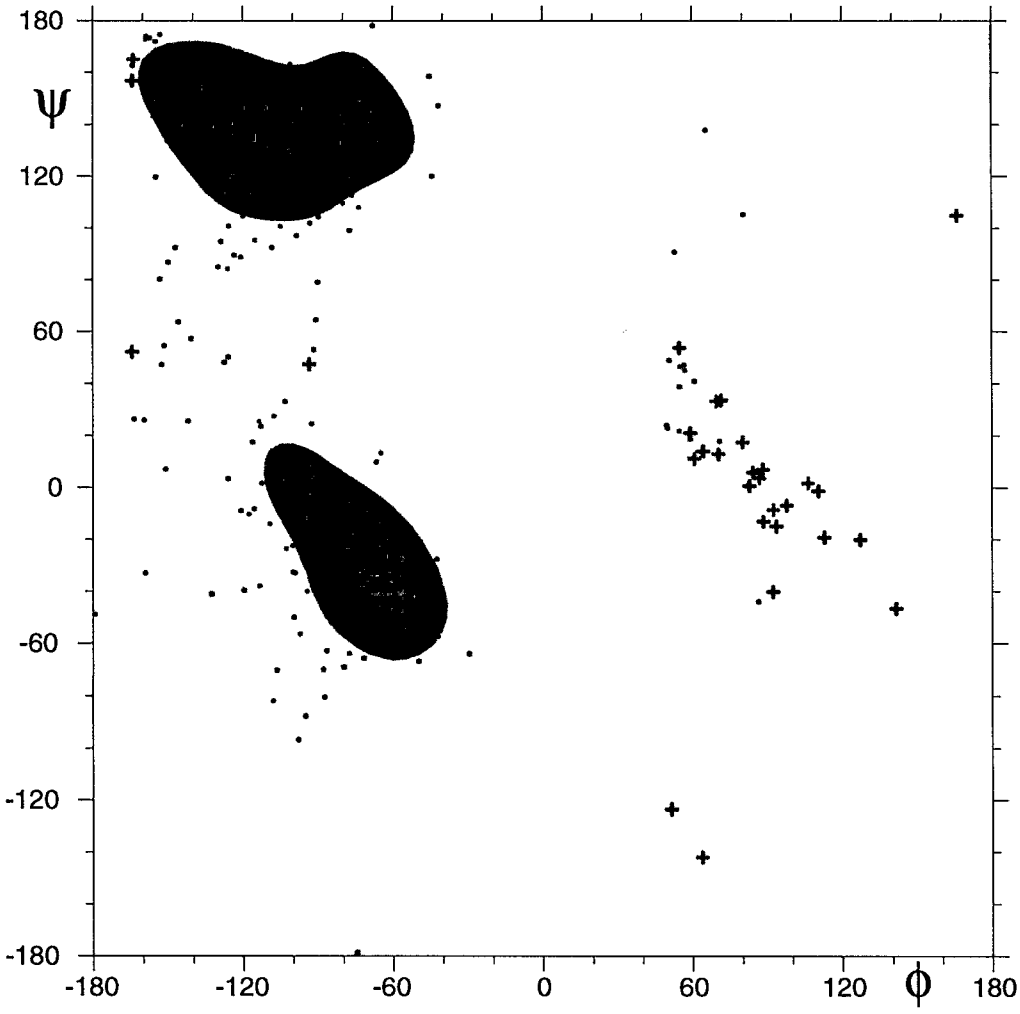
ψ
120
60
0
-60
-120
-180
-180
-120
-60
0
60
120
ϕ
180


180
ψ
120
60
0
-60
-120
-180
-180
-120
-60
0
60
120
ϕ
180


C
N