The NMR solution structure of subunit F of the methanogenic A_1A_O ATP synthase and its interaction with the nucleotide-binding subunit B

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[1] Section of Structure and Function of Molecular Motors

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Supplemental Figure Legends

Figure S1. Amino acid sequence of the F subunit with a survey of the short- and medium-range NOE connectivities, which were used to establish the sequence-specific ^{1}H NMR assignment and to identify elements of regular secondary structure.

Figure S2. 2D ^{1}H-^{15}N HSQC of F subunit with different peak shapes and intensities are indicating chemical exchange phenomena. The unlabelled peaks are single sharp resonances having line-width of about 25-30 Hz. The peaks marked in single letter amino acid residue with asterisks indicate residues undergoing chemical exchange. The peaks marked in single letter amino acid residue with subscripts *a* and *b* indicate multiple peaks for the same residue. For example, A35, K101, and V45 have multiple peaks and are marked with subscripts *a* and *b*.

Figure S3. 1D projection of representative ^{1}H-^{15}N HSQC peaks of F subunit are plotted in the same Hz/pt scale. The column 1 shows single sharp peaks, column 2 single peak with exchange broadening and column 3 shows two or more peaks for the same residue. The residue along with the sequence number is marked in the left side of the peak.

Figure S4: Bar diagram showing intensities of the HSQC cross peaks as a function of residue position of the F subunit. Intensities were measured using SPARKY. Intensity of peaks could not be obtained for residues because of signal overlap are no assignments were made.

Figure S5: Schematic representation of the secondary structure of subunit F is shown. Dotted lines indicate interstrand hydrogen bonds and solid lines indicate long-range ^{1}H-^{1}H distances in 4 parallel β-strands of the F subunit.

Figure S1


10
20
30
40
MELAVIGKSEFVTGFRLAGISKVYETPDIPATESAVRSVL
$d_{NN}(i,i+1)$
$d_{\alpha N}(i,i+1)$
$d_{\beta N}(i,i+1)$
$d_{NN}(i,i+2)$
$d_{\alpha N}(i,i+2)$
$d_{\alpha N}(i,i+3)$
$d_{\alpha\beta}(i,i+3)$
$d_{\alpha N}(i,i+4)$
50
60
70
80
EDKSVGILVMHNDDIGNLPEVLRKNLNESVQPTVVALGGS
$d_{NN}(i,i+1)$
$d_{\alpha N}(i,i+1)$
$d_{\beta N}(i,i+1)$
$d_{NN}(i,i+2)$
$d_{\alpha N}(i,i+2)$
$d_{\alpha N}(i,i+3)$
$d_{\alpha\beta}(i,i+3)$
$d_{\alpha N}(i,i+4)$
90
100
GSGSTSLREKIKQAVGVDLWK
$d_{NN}(i,i+1)$
$d_{\alpha N}(i,i+1)$
$d_{\beta N}(i,i+1)$
$d_{NN}(i,i+2)$
$d_{\alpha N}(i,i+2)$
$d_{\alpha N}(i,i+3)$
$d_{\alpha\beta}(i,i+3)$
$d_{\alpha N}(i,i+4)$

Figure S2

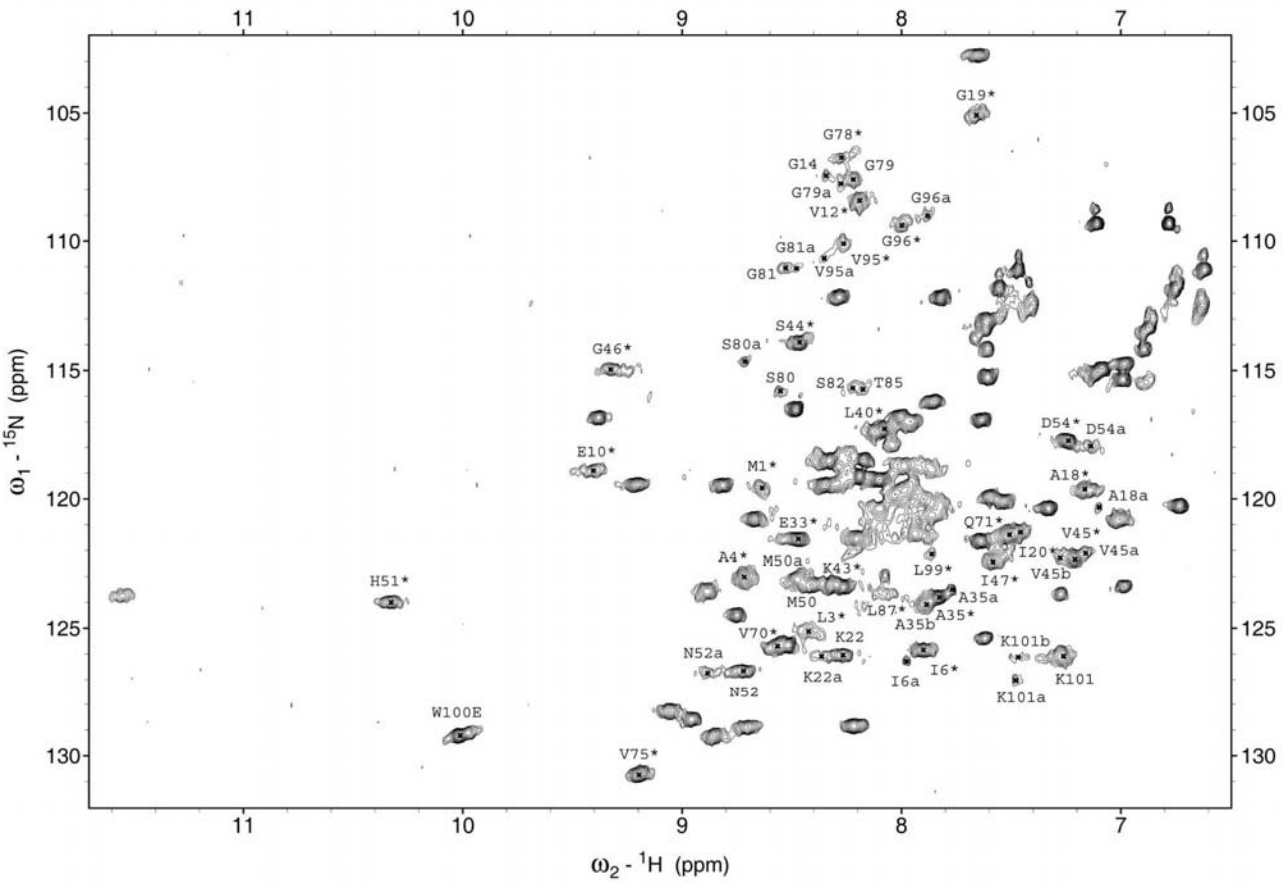

11
10
9
8
7
105
110
115
120
125
130
ω_1 - ^{15}N (ppm)
ω_2 - ^{1}H (ppm)
G19*
G78*
G14
G79
G79a
V12*
G96a
G96*
G81a
V95*
G81
V95a
S44*
S80a
G46*
S80
S82
T85
L40*
D54*
D54a
E10*
M1*
A18*
A18a
E33*
Q71*
V45*
A4*
M50a
K43*
I20*
V45a
L99*
I47*
V45b
H51*
M50
A35a
L87*
A35*
L3*
A35b
V70*
K22
K101b
N52a
K22a
I6a
I6*
K101
N52
K101a
W100E
V75*

Figure S3

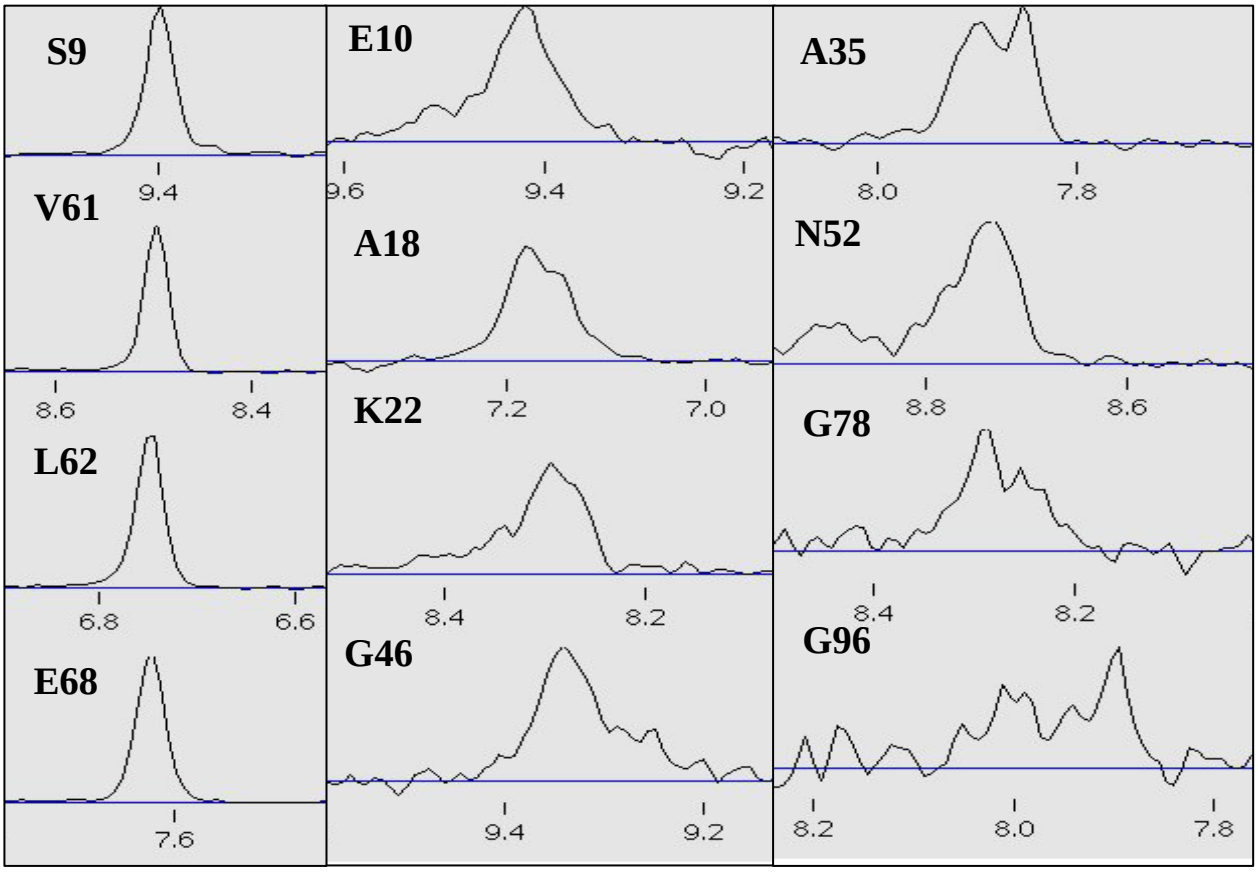

S9
9.4
E10
9.6
9.4
9.2
A35
8.0
7.8
V61
8.6
8.4
A18
7.2
7.0
N52
8.8
8.6
L62
6.8
6.6
K22
8.4
8.2
G78
8.4
8.2
E68
7.6
G46
9.4
9.2
G96
8.2
8.0
7.8

Figure S4

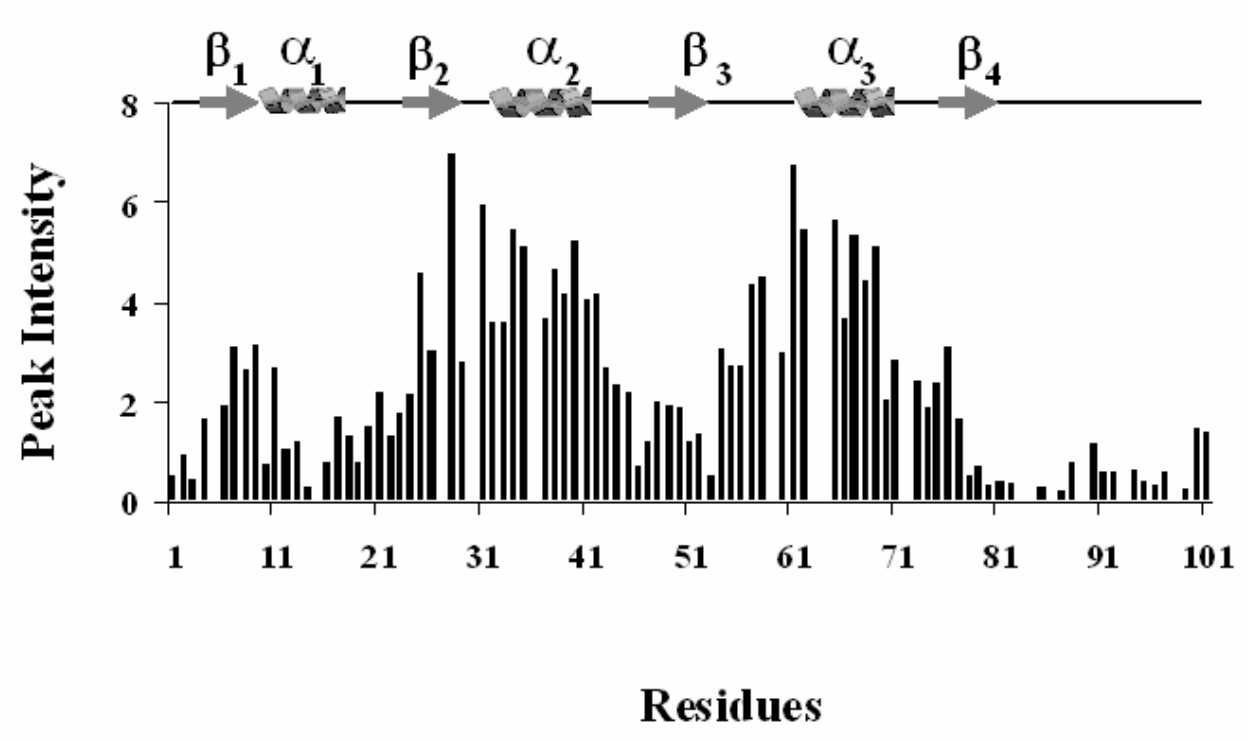
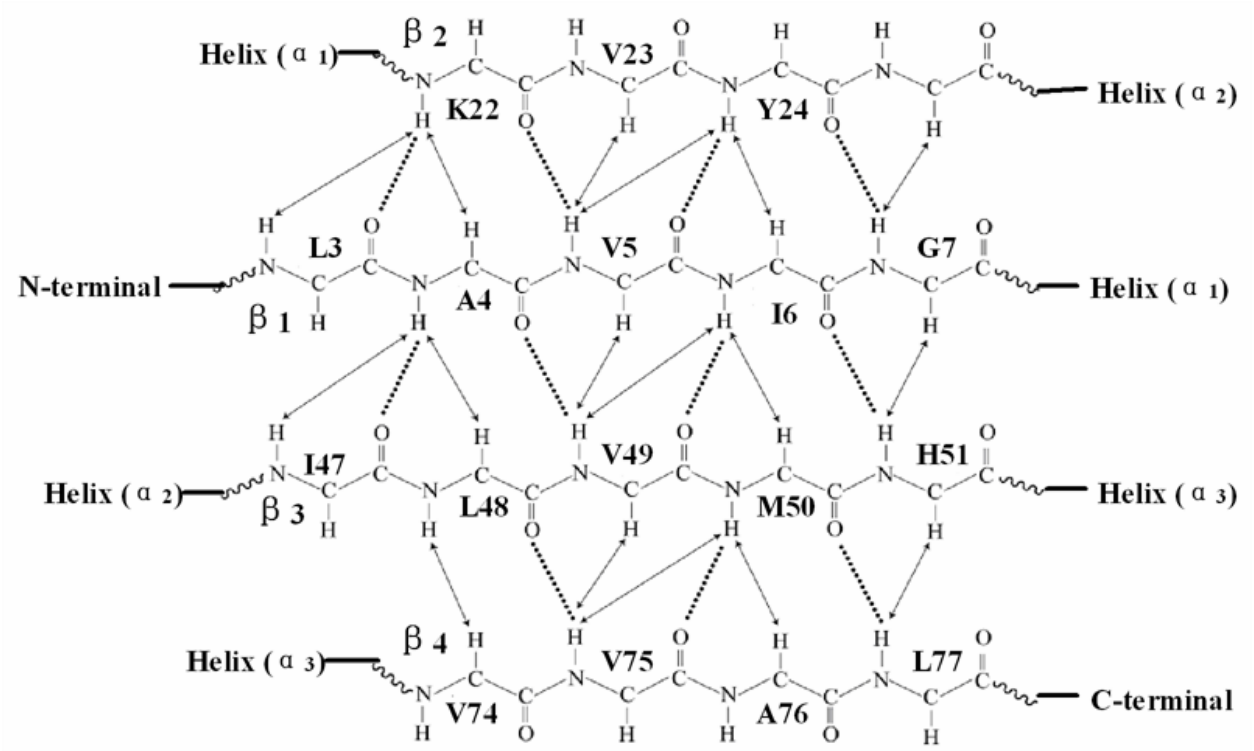

β1
α1
β2
α2
β3
α3
β4
Peak Intensity
0
2
4
6
8
1
11
21
31
41
51
61
71
81
91
101
Residues

Figure S5


Helix (α 1)
β 2
V23
K22
Y24
Helix (α 2)
N-terminal
L3
V5
G7
A4
I6
β 1
Helix (α 1)
Helix (α 2)
I47
V49
H51
L48
M50
β 3
Helix (α 3)
Helix (α 3)
β 4
V75
L77
V74
A76
C-terminal