Supporting Information for:

Atomic Resolution Structure of Monomorphic $A\beta_{42}$ Amyloid Fibrils

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The MPL measurements were performed on 4 grids: undiluted U-^{13}C/^{15}N-Aβ_{M01-42} taken from an NMR sample, 3x dilution, 10x dilution and an extra 10x dilution which had too much ice to load in the freeze dry. The last grid was warmed, blotted to remove extra water and re-frozen. All four were freeze dried. The undiluted sample showed no isolated filaments. The other grids had thin straight filaments ~2.5+/-15% kDa/A and thicker sometimes twisted filaments ~4.5+/-10% kDa/A in addition to TMV. After extensive searching the samples revealed some fairly clean areas. The TMV M/L varied considerably from area to area, due to salt and did not correlate with filament M/L so we did not try to re-normalize the mass calibration to give 13.1 kDa/A. The ~2.5kDa/A filaments are in the minority and appear to be twisted. The dominant species is the ~5kDa/A filament that is clearly twisted and sometimes separated into parallel strands.

In addition to the ~2.5 and ~4.9 kDa/Å filaments, there were a few very thin filaments with M/L ~1.3kDa/A and a few with M/L ~7.5 kDa/A. In some cases the thick filaments appear to be made up of two thin filaments side-by-side with a cleft between them. Often there were abrupt transitions where one of the "pair" would terminate. All appeared to have blunt ends.

The mass meaurements were performed with PCMass32 available on ftp.stem.bnl.gov used for automatically selecting particles and viewing blemishes (in the image minus model display). The measurement proceeds in 5 steps:

1. The program masks out objects significantly above background noise and measures the background level in the remaining areas and the dose (via counting statistics).

2. A threshold (based on model) is set and the program traces the perimeter of areas above the threshold, comparing to max & min diameters (or length) of the model.

3. Models appropriate for an area are refined against the image data (centering, size, amplitude, orientation, twist, curvature, etc.) and areas satisfying selection criteria are submitted for mass, M/L or M/Area measurement. All model parameters, fitting parameters and measurements are stored in a file nkxxxxyy.SMM (STEM Mass Measurement) which is read back in whenever the image nkxxxxyy.dat is viewed.

4. An operator steps through each measurement to judge quality. For short filaments the measuring rectangle may extend past the end of the filament. The image may have bright spots (salt or heavy atoms) or "blemishes" that are evident in the image minus model display. Those measurements are deleted by changing the mass value to negative (that can be change back to positive later if a mistake was made). Areas missed by the automatic selection can be entered manually.

5. A database program reads the nkxxxxyy.SMM files in a specified range and computes mean, SD and N for each model in that file, as well as global averages and histograms. If the background and TMV are of high quality, the program can scale the mass calibration to give TMV=13.1 kDa/A.

For a clean specimen with good preservation, the accuracy is determined by counting statistics and fluctuations in substrate thickness. At a dose of 10el/A**2 the TMV SD is expected to be <2% and the 2.5 kDa/A filament <5%. That is achieved in many of the Aβ_{M01-42} images, but the fluctuation from one image to another is larger than expected due to background residue. Salt deposits tend to accumulate in the crevice where the TMV (which is very rigid) touches the substrate. Therefore a high TMV value is usually a reliable indicator of salt or other problems. The radial density profile of the TMV can be significantly altered and the central hole filled in. Thin filaments may be less rigid and flattened so they do not accumulate residue to the same extent, making scaling for TMV value incorrect. A useful indicator of overall quality is the SD of the means for individual images.

An additional problem with your data is the strong tendency of your filaments to attract heavy atom bright spots. This has been seen before with α-synuclein and may indicate specific binding. It is not present in TMV particles in the same image. It may increase the M/L of thin filaments by as much as 5%.

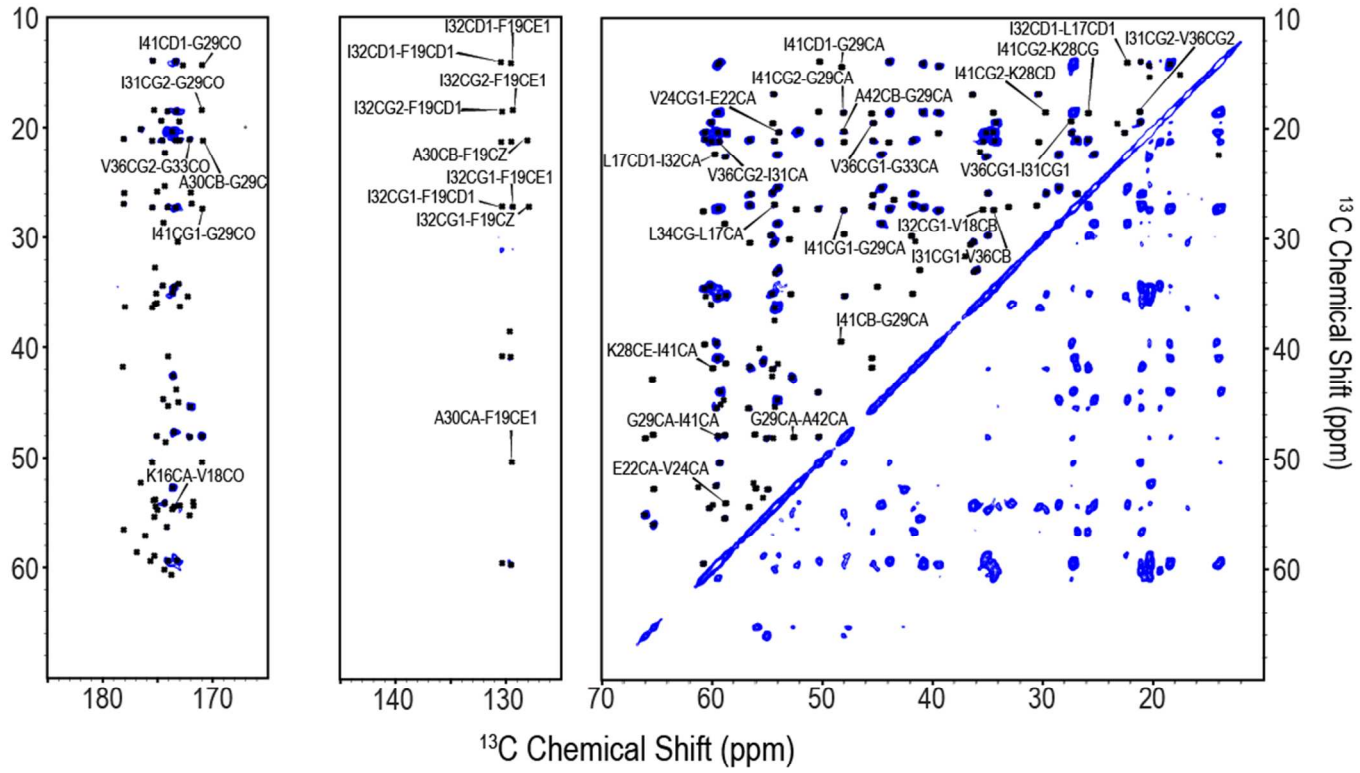

Figure S1. 2D ^{13}C-^{13}C MAS PAR spectrum of 30 % U-^{13}C/^{15}N-A$\beta_{M01\text{-}42}$ fibrils recorded at $\omega_{0H}/2\pi$=800MHz, T=277K, $\omega_r/2\pi$=20kHz. τ_{mix}=20 ms, and $\omega_{1H}/2\pi$ = 83 kHz decoupling field. For optimal PAR mixing, the radio frequency (RF) fields were set to $\omega_{13C}/2\pi$=62.5 kHz and $\omega_{1H}/2\pi$=55 kHz on the on the ^{13}C and ^{1}H channels, respectively.

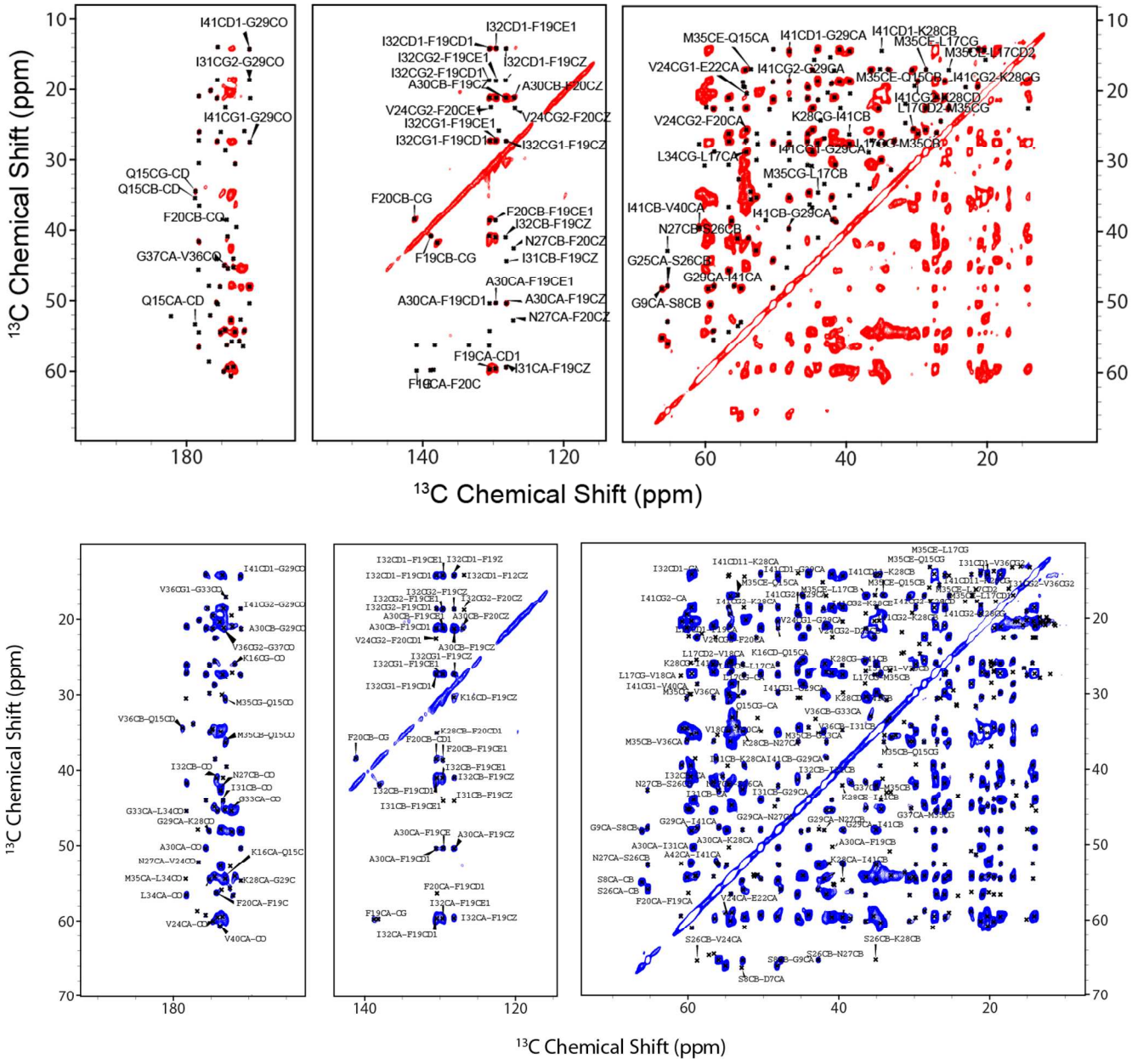

Figure S2. 2D ^{13}C-^{13}C MAS PAR spectrum of U-^{13}C/^{15}N-A$\beta_{M01\text{-}42}$ fibrils recorded at $\omega_{0H}/2\pi$=800MHz, T=277K, $\omega_r/2\pi$=20kHz. τ_{mix}= (a) 5 ms (shown in red) and (b)10 ms (shown in blue), and $\omega_{1H}/2\pi$ = 83 kHz decoupling field. For optimal PAR mixing, the radio frequency (RF) fields were set to $\omega_{13C}/2\pi$=62.5 kHz and $\omega_{1H}/2\pi$=55 kHz on the on the ^{13}C and ^{1}H channels, respectively. Several important inter-residue cross peaks are denoted with red labels in the expanded region of the spectrum.

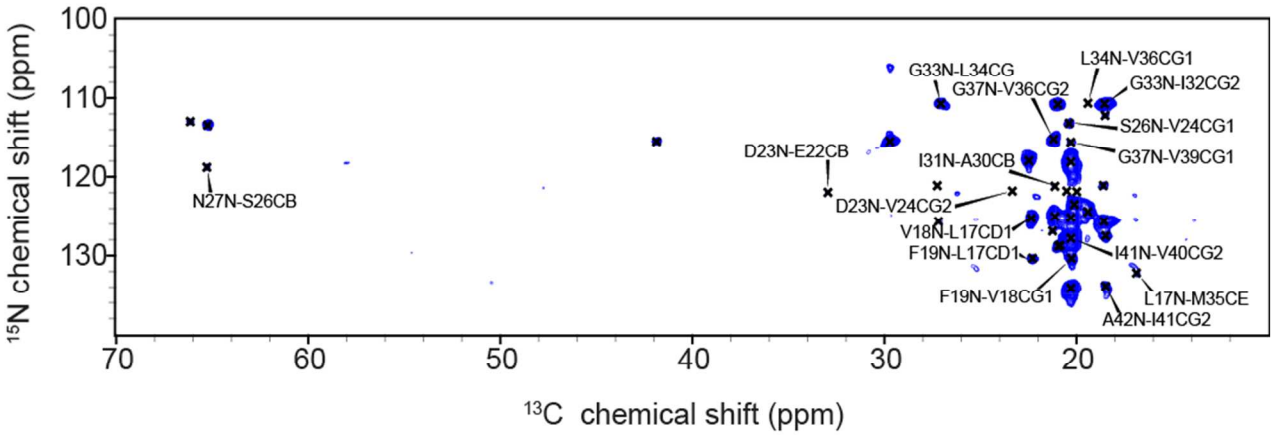

Figure S3. 2D ZF-TEDOR spectrum of 1,6$^{13}C_2$-glucose labeled $A\beta_{M01\text{-}42}$ fibrils recorded at 800 MHz, $\omega_r/2\pi$=20.0 kHz, VT gas regulated to 277 K with 83 kHz TPPM during acquisition.

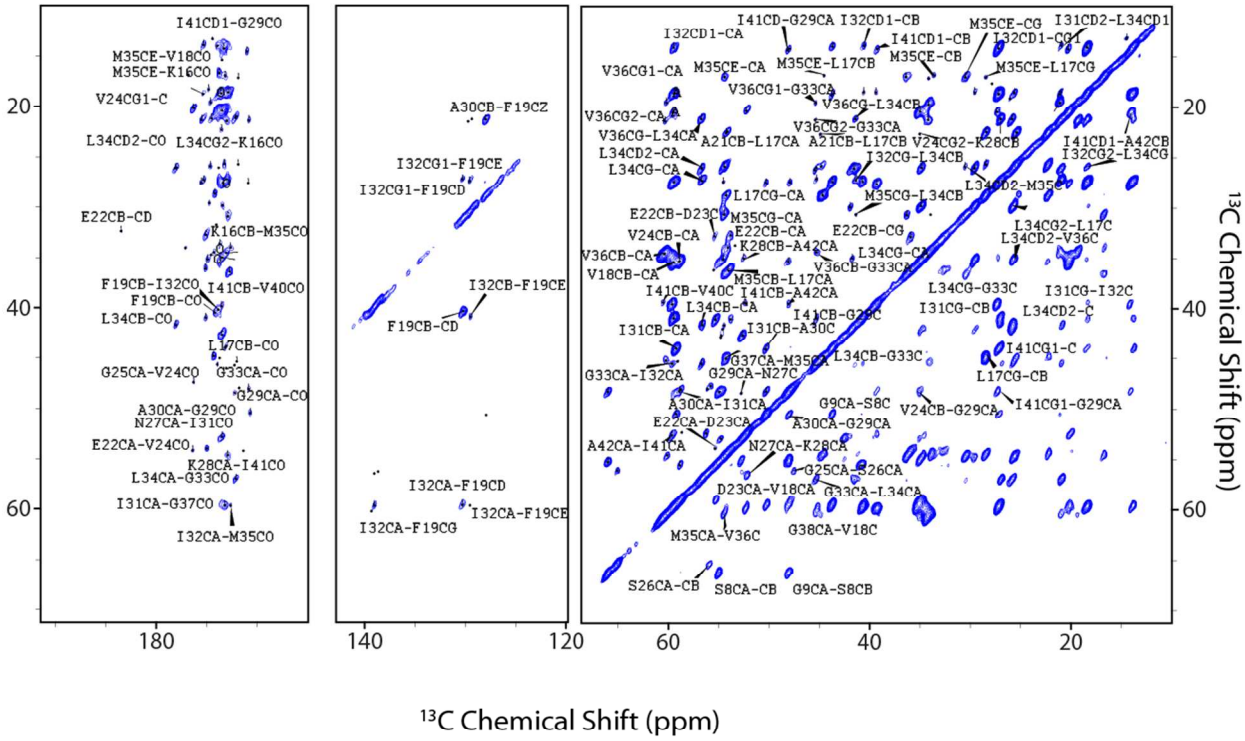

Figure S4. 2D ^{13}C-^{13}C MAS PAR spectrum of [2-$^{13}C_1$ glycerol/1,3-$^{13}C_2$ glycerol mixed sample]/^{15}N-Aβ_{M01-42} fibrils recorded at $\omega_{0H}/2\pi$=800MHz, T=277K, $\omega_r/2\pi$=20kHz. τmix=20 ms, and $\omega_{1H}/2\pi$ = 83 kHz decoupling field. For optimal PAR mixing, the radio frequency (RF) fields were set to $\omega_{13C}/2\pi$=62.5 kHz and $\omega_{1H}/2\pi$=55 kHz on the on the ^{13}C and ^{1}H channels, respectively.

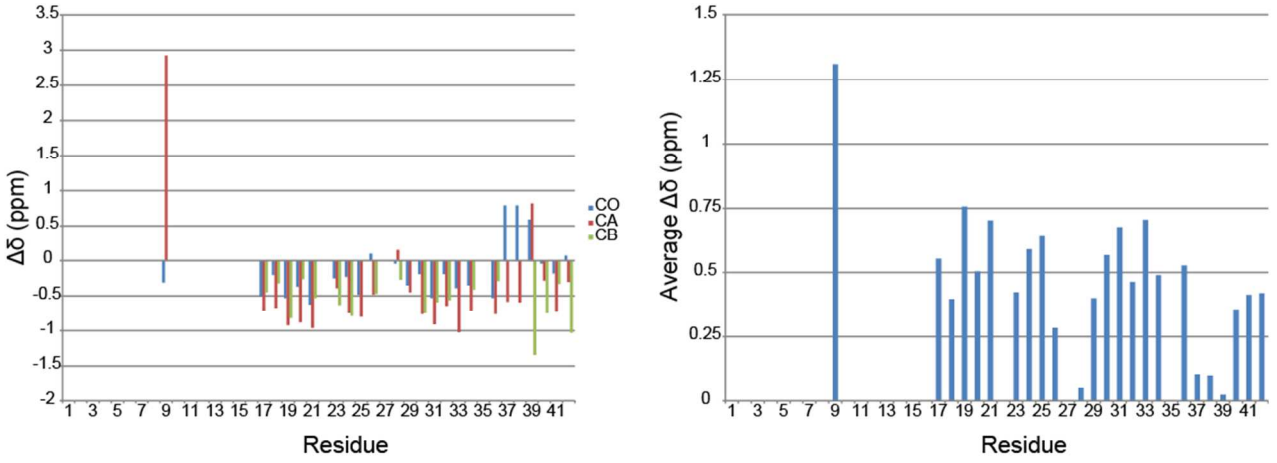

Figure S5. Comparison of chemical shifts for residues observed by Ishii alongside those reported by us previously.

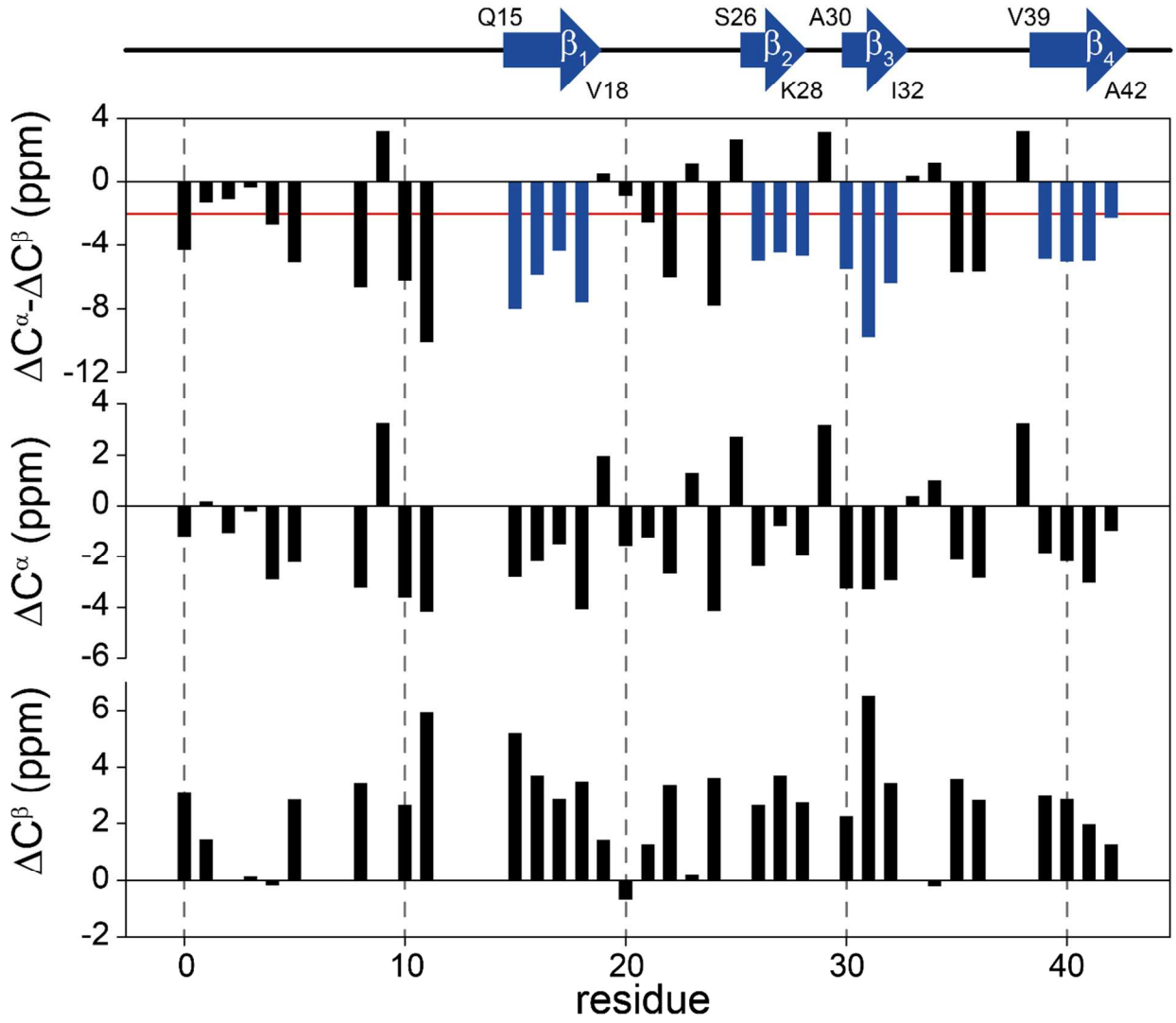

Figure S6. Secondary chemical shifts of C^{α} and C^{β} sites of each residue. The upper plot shows the difference between the secondary chemical shifts of C^{α} and C^{β} sites. Three or more consecutive sites where this difference is less than -2 (red line) indicate the presence of a β-strand. These bars are shown in blue.

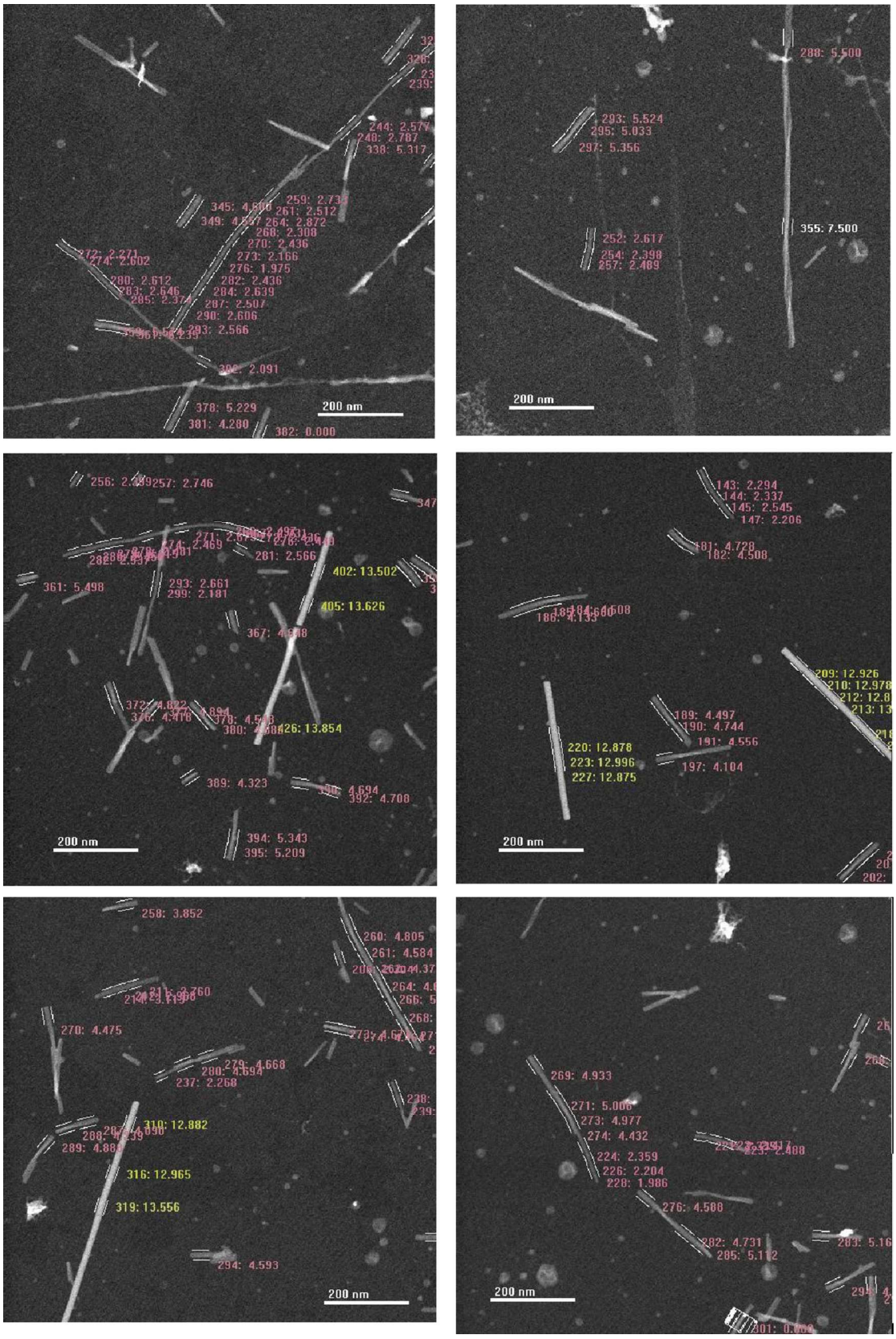

Figure S7. Additional micrographs from STEM

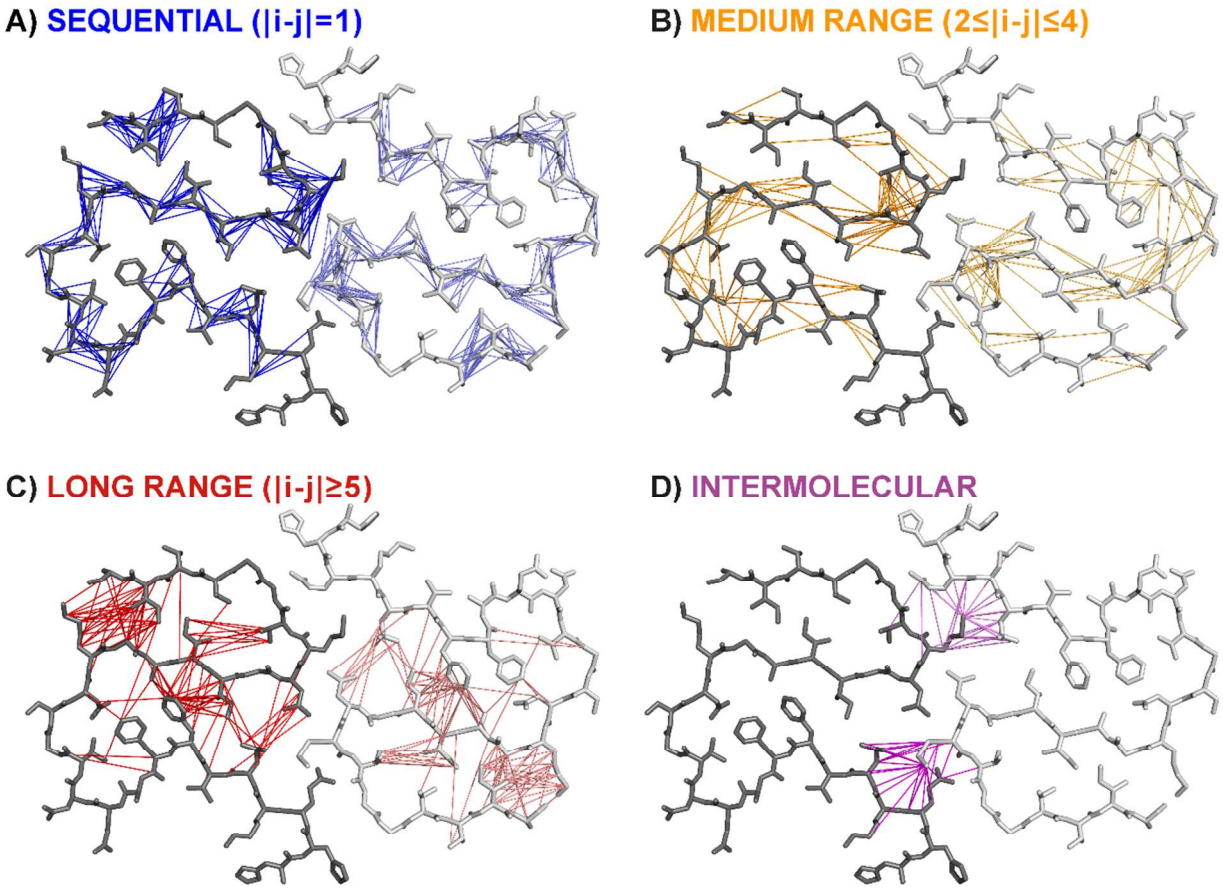

Figure S8. Constraints for structure calculation. Schematic representation of unique constraints used for structure calculation. A total of 487 unique distance constraints of which (A) 264 were sequential contacts, (B) 93 medium range, (C) 104 long range, and (D) 26 intermolecular distance constraints.

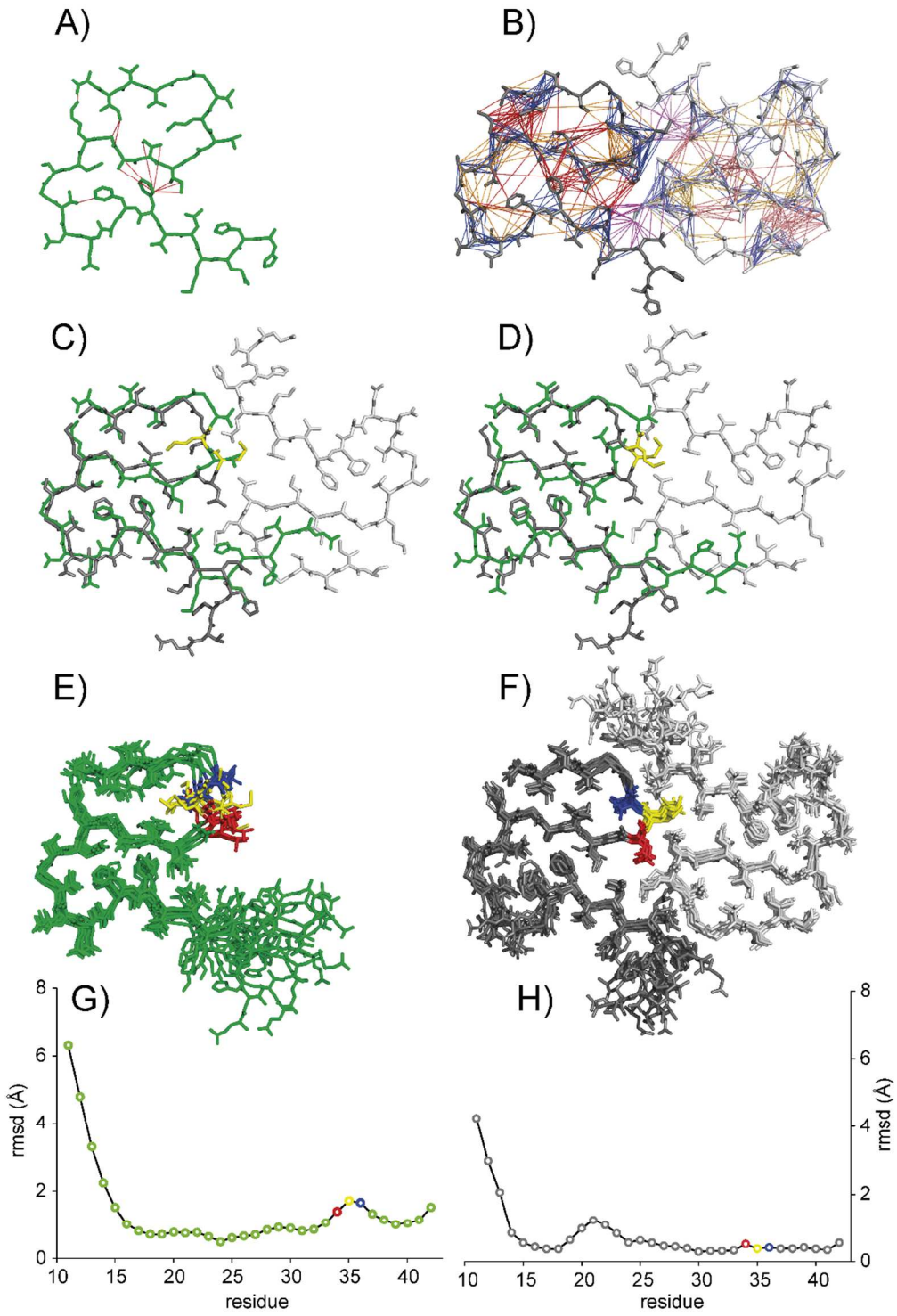

Figure S9. Comparison between the structural model proposed by Xiao et al. and the structure presented here. **(A)** Schematic representation of unique constraints used for structure calculation. A total of 38 unique distance constraints of which 11 were long range distance constraints. **(B)** Schematic representation of unique constraints used for structure calculation. A total of 487 unique distance constraints of which 264 were sequential contacts, 93 medium range, 104 long range, and 26 intermolecular distance constraints. **(C+D)** Alignment of chain F of Ishii's structural model with chain E of the structure presented here. The lowest (C) and second lowest (D) energy models Ishii's structural model are compared to the lowest energy model of the structure presented here. **(E)** Bundle of the 10 lowest energy models of Ishii's structural model. (F) Bundle of the 10 lowest energy models of the structure presented here. Residue-wise RMSD is shown for Ishii's structural model **(G)** and the structure presented here **(H)**.

TABLE S1 - Total number of picked intraresidual, sequential, medium range, long range, and intermolecular contacts.

	INTRA	SEQUENTIAL	MEDIUM	LONG	INTER
100%UCN-PAR-5ms	74	63	8	34	10
100%UCN-PAR-10ms	119	102	25	51	12
100%UCN-PAR-20ms	103	122	33	66	18
100%UCN-PAIN-30ms	38	35	26	15	1
100%UCN-DARR-25ms	129	36	1	5	0
30%UCN-DARR-100ms	146	121	4	10	0
30%UCN-PAR-20ms	125	74	7	30	0
1,6Glc-TEDOR-6.4ms	26	10	1	0	0
1,6Glc-TEDOR-12ms	18	11	4	0	1
1,6Glc-DARR-100ms	41	1	2	2	0
2Gly-DARR-400ms	51	40	8	6	0
FS-REDOR	0	0	0	1	0
TOTAL	**870**	**615**	**119**	**220**	**42**

TABLE S2 Table of UNIQUE sequential, medium range, long range, and intermolecular contacts.

A = 100%UCN-PAR-5ms - 8.5 Angstroms
B = 100%UCN-PAR-10ms - 8.5 Angstroms
C = 100%UCN-PAR-20ms - 10.0 Angstroms
D = 100%UCN-PAIN-30ms - 12.0 Angstroms
E = 100%UCN-DARR-25ms - 7.5 Angstroms
F = 30%UCN-DARR-100ms - 7.5 Angstroms
G = 30%UCN-PAR-20ms - 10.0 Angstroms
H = 1,6Glc-TEDOR-6.4ms - 6.5 Angstroms
I = 1,6Glc-TEDOR-12ms - 7.5 Angstroms
J = 1,6Glc-DARR-100ms - 7.5 Angstroms
K = 2Gly-DARR-400ms - 8.0 Angstroms
L = FS-REDOR - 4.7 Angstroms

(X = observed, # = count)
(Types (T): S=SEQ, M=MED, L=LONG, X=INTER)

NUC1	NUC2	A	B	C	D	E	F	G	H	I	J	K	L	#	T	RESTRAINT
Q15CA	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
Q15CB	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
Q15CG	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
Q15CG	K16CD	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
Q15CO	K16CA	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
Q15CA	K16CD	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
Q15CG	**M35CB**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
Q15CO	**M35CB**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
Q15CO	**M35CG**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
Q15CD	**V36CB**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
Q15CD	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
Q15CO	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
Q15CD	**M35N**	**-**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**12.0**
Q15CO	K16CD	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
K16CO	L17CA	X	-	X	-	X	X	X	-	-	-	-	-	5	S	7.5
K16CD	L17CA	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
K16CO	L17CD1	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
K16CO	L17CB	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
K16CD	L17CD2	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
K16CO	L17CD2	-	-	X	-	X	X	-	-	-	-	-	-	3	S	7.5
K16CO	L17CG	-	-	X	-	-	X	-	-	-	-	X	-	3	S	7.5
K16CD	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
K16CO	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
K16CG	L17N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
K16CO	L17N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
K16CB	V18N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
K16CO	V18N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
K16CO	L17CO	-	-	-	-	X	-	-	-	-	-	X	-	2	S	7.5
K16CB	L17CD2	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
K16CA	V18CO	-	-	-	-	-	-	X	-	-	-	-	-	1	M	10.0
L17CG	V18CA	X	X	X	-	-	X	X	-	-	-	X	-	6	S	7.5

L17CD1	I32CD1	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
L17CD2	**M35CG**	**X**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**2**	**X**	**8.5**
L17CG	**M35CB**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
L17CA	L34CG	X	X	-	-	-	-	X	-	-	-	-	-	3	L	8.5
L17CB	**M35CB**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
L17CB	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
L17CD2	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
L17CG	**M35CE**	**X**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**3**	**X**	**8.5**
L17CB	**M35CG**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**8.5**
L17CD2	V18CA	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
L17CD1	F19CA	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
L17CD1	**M35CE**	**-**	**X**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**2**	**X**	**8.5**
L17CA	V18CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
L17CB	V18CA	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
L17CD1	V18CA	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
L17CG	V18CB	-	-	X	-	-	-	-	-	-	-	X	-	2	S	8.0
L17CD1	F19CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
L17CD1	L34CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CD1	L34CG	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CD1	**M35CB**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
L17CD1	**M35CG**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
L17CD2	**M35CB**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
L17CG	I32CA	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CD2	I32CD1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CG	L34CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CG	L34CG	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
L17CA	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
L17CO	**M35CE**	**-**	**-**	**X**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**1**	**X**	**10.0**
L17CA	V18N	-	-	-	X	-	-	-	X	-	-	-	-	2	S	6.5
L17CB	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
L17CD1	V18CB	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
L17CA	V18CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L17CD1	V18CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L17CA	V18CG1	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L17CB	V18CG1	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L17CD1	I32CA	-	-	-	-	-	X	X	-	-	-	-	-	2	L	7.5
L17CD1	V18N	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
L17CD1	F19N	-	-	-	-	-	-	-	-	X	-	-	-	1	M	7.5
L17N	**M35CE**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**-**	**X**	**-**	**-**	**-**	**1**	**X**	**7.5**
L17CG	F19CA	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
V18CB	F19CD1	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
V18CB	F20CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
V18CA	A21CB	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
V18N	L34CD2	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
V18CB	I32CG1	-	-	-	-	-	-	X	-	-	-	-	-	1	L	10.0
V18CG1	F19N	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
V18CA	F19CO	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
V18CO	F20CA	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
F19CA	F20CG	X	-	-	-	-	-	-	-	-	-	-	-	1	S	8.5
F19CG	F20CA	X	-	-	-	-	X	-	-	-	-	X	-	3	S	7.5
F19CE1	F20CB	X	X	-	-	-	-	X	-	-	-	-	-	3	S	8.5
F19CD1	A30CA	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
F19CE1	A30CA	X	X	X	-	-	-	X	-	-	-	X	-	5	L	8.0
F19CZ	A30CA	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5

F19CZ	A30CB	X	X	X	-	X	-	X	-	-	-	-	-	5	L	7.5
F19CZ	I31CA	X	-	-	-	-	-	-	-	-	-	-	-	1	L	8.5
F19CZ	I31CB	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
F19CZ	I32CB	X	X	-	-	-	-	-	-	-	-	-	-	2	L	8.5
F19CD1	I32CD1	X	X	X	-	-	X	X	-	-	-	-	-	5	L	7.5
F19CE1	I32CD1	X	X	X	-	-	X	X	-	-	-	X	-	6	L	7.5
F19CZ	I32CD1	X	X	-	-	-	-	-	-	-	-	-	-	2	L	8.5
F19CD1	I32CG1	X	X	X	-	-	X	X	-	-	X	-	-	6	L	7.5
F19CE1	I32CG1	X	X	X	-	-	X	X	-	-	-	-	-	5	L	7.5
F19CZ	I32CG1	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
F19CD1	I32CG2	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
F19CE1	I32CG2	X	X	-	-	-	-	X	-	-	-	-	-	3	L	8.5
F19CZ	I32CG2	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
F19CA	F20CA	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
F19CG	F20CG	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
F19CD1	F20CA	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
F19CO	F20CA	-	X	X	-	X	-	-	-	-	-	-	-	3	S	7.5
F19CB	A30CA	-	X	-	-	-	-	-	-	-	-	-	-	1	L	8.5
F19CD1	A30CB	-	X	X	-	-	X	-	-	-	X	-	-	4	L	7.5
F19CE1	A30CB	-	X	X	-	X	X	-	-	-	-	-	-	4	L	7.5
F19CE1	I31CB	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
F19CD1	I32CA	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
F19CE1	I32CA	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
F19CZ	I32CA	-	X	-	-	-	-	-	-	-	-	-	-	1	L	8.5
F19CD1	I32CB	-	X	X	-	X	-	-	-	-	-	-	-	3	L	7.5
F19CE1	I32CB	-	X	X	-	-	-	-	-	-	-	X	-	3	L	8.0
F19CB	I31CO	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
F19CD1	I31CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
F19CE1	I31CG2	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
F19CA	F20N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
F19CB	F20N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
F19CZ	N27CB	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F19N	I32CO	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F19CZ	A30N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F19CB	I32N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F19CD1	I32N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F19CB	F20CA	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
F19CG	I32CB	-	-	-	-	X	-	-	-	-	-	-	-	1	L	7.5
F20CA	V24CG2	X	X	X	-	-	-	-	-	-	-	-	-	3	M	8.5
F20CE1	V24CG2	X	-	-	-	-	-	-	-	-	-	-	-	1	M	8.5
F20CZ	V24CG2	X	-	-	-	-	-	-	-	-	-	-	-	1	M	8.5
F20CZ	N27CA	X	-	-	-	-	-	-	-	-	-	-	-	1	L	8.5
F20CZ	N27CB	X	-	-	-	-	-	-	-	-	-	-	-	1	L	8.5
F20CZ	A30CB	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
F20CD1	V24CG2	-	X	-	-	-	-	-	-	-	X	-	-	2	M	7.5
F20CA	A21CA	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
F20CB	E22CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
F20CA	V24CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
F20CA	A21N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
F20CD1	E22CA	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
F20CA	E22N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
F20CA	G25N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F20CO	G25N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
F20CO	A21CA	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5

F20CA	A21CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
F20CA	A21CB	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CA	E22CB	-	X	-	-	-	X	-	-	-	-	-	-	2	S	7.5
A21CA	V24CG2	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
A21CB	E22N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
A21CB	E22CB	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CB	E22CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CO	E22CD	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CO	E22CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CO	E22CB	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
A21CA	E22CD	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
E22CA	V24CG1	X	-	-	-	-	-	X	-	-	-	-	-	2	M	8.5
E22CA	V24CA	-	X	X	-	-	-	X	-	-	-	-	-	3	M	8.5
E22CG	D23CG	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
E22CA	D23CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
E22CA	D23CG	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
E22CA	D23CO	-	-	-	-	-	X	-	-	-	X	-	-	2	S	7.5
E22CB	D23CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
E22CB	D23CO	-	-	-	-	-	X	X	-	-	-	X	-	3	S	7.5
E22CG	D23CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
E22CO	D23CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
E22CB	D23CB	-	-	-	-	-	-	X	-	-	-	-	-	1	S	10.0
E22CO	D23CG	-	-	-	-	-	-	X	-	-	-	X	-	2	S	8.0
E22CA	D23N	-	-	-	-	-	-	-	X	-	-	-	-	1	S	6.5
E22CB	D23N	-	-	-	-	-	-	-	-	X	-	-	-	1	S	7.5
D23CB	V24CG2	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
D23N	V24CB	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
D23N	G25CA	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
D23CA	V24CA	-	-	-	-	-	X	X	-	-	-	X	-	3	S	7.5
D23CA	V24CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
D23CB	V24CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
D23CG	V24CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
D23CO	V24CG2	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
D23CB	V24CA	-	-	-	-	-	-	X	-	-	-	-	-	1	S	10.0
D23N	V24CG2	-	-	-	-	-	-	-	-	X	-	-	-	1	S	7.5
D23CO	V24CA	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
D23CO	V24CB	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
V24CA	G25CA	X	X	-	-	-	X	X	-	-	-	-	-	4	S	7.5
V24CO	G25CA	X	X	-	-	X	X	-	-	-	-	-	-	4	S	7.5
V24CG1	G25CA	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
V24CA	S26CB	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
V24CO	N27CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
V24CB	S26CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
V24CG2	N27CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
V24CA	S26CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
V24CO	G25N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V24CB	K28N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
V24CG2	A30N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
V24CO	G25CO	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
V24CB	S26CO	-	-	-	-	-	-	X	-	-	-	-	-	1	M	10.0
V24CG1	S26N	-	-	-	-	-	-	-	-	X	-	-	-	1	M	7.5
V24CB	G25CA	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
G25CA	S26CA	X	X	X	-	-	X	X	-	-	-	X	-	6	S	7.5
G25CA	S26CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5

G25CO	S26CA	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
G25CO	S26CB	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
S26CB	N27CA	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
S26CO	N27CA	X	X	-	-	X	X	-	-	-	-	-	-	4	S	7.5
S26CB	N27CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
S26CA	N27CA	-	X	X	-	-	-	X	-	-	-	-	-	3	S	8.5
S26CA	N27CB	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
S26CB	K28CB	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
S26CA	N27CO	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
S26CB	K28CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
S26CO	G29CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
S26CB	N27N	-	-	-	X	-	-	-	-	X	-	-	-	2	S	7.5
S26N	K28CB	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
S26CA	G29N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
S26CB	N27CO	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
S26CO	N27CB	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
N27CA	K28CA	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
N27CA	K28CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
N27CA	K28CD	X	X	X	-	-	-	X	-	-	-	-	-	4	S	8.5
N27CA	K28CG	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
N27CO	K28CB	-	X	-	-	-	X	-	-	-	-	-	-	2	S	7.5
N27CO	K28CD	-	X	X	-	-	-	-	-	-	-	X	-	3	S	8.0
N27CA	G29CA	-	X	X	-	-	X	-	-	-	-	-	-	3	M	7.5
N27CB	G29CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
N27CB	K28CB	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
N27CO	K28CG	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
N27CA	A30CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
N27N	K28CA	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
N27CA	G29N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
N27CA	A30N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
N27CO	A42N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
N27CA	K28CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
N27CB	K28CA	-	-	-	-	-	X	-	-	-	-	X	-	2	S	7.5
N27CB	K28CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
N27CO	K28CA	-	-	-	-	-	-	X	-	-	-	X	-	2	S	8.0
N27CO	G29CA	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
K28CB	G29CA	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
K28CD	G29CA	X	X	X	-	-	-	X	-	-	-	-	-	4	S	8.5
K28CE	G29CA	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
K28CG	G29CA	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
K28CA	G29CA	X	X	X	-	-	X	X	-	-	-	X	-	6	S	7.5
K28CO	G29CA	X	X	X	-	X	X	X	-	-	-	X	-	7	S	7.5
K28CG	I41CB	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
K28CB	I41CD1	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
K28CD	I41CG2	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
K28CG	I41CG2	X	X	-	-	-	-	X	-	-	-	-	-	3	L	8.5
K28CA	G29CO	-	X	X	-	-	X	-	-	-	-	-	-	3	S	7.5
K28CB	A30CA	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
K28CA	A30CA	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
K28CA	I41CB	-	X	-	-	-	-	-	-	-	-	-	-	1	L	8.5
K28CD	I41CB	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CE	I41CB	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CG	I41CA	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CA	I41CD1	-	X	-	-	-	-	-	-	-	-	-	-	1	L	8.5

K28CG	I41CD1	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CA	I41CG2	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CB	I41CG2	-	X	-	-	-	-	-	-	-	-	-	-	1	L	8.5
K28CE	I41CG2	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
K28CB	G29CO	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
K28CD	G29CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
K28CE	G29CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
K28CG	G29CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
K28CB	I41CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CD	I41CA	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CE	I41CA	-	-	X	-	-	-	X	-	-	-	-	-	2	L	10.0
K28CE	I41CO	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CD	I41CD1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CE	I41CD1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CD	I41CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
K28CA	G29N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
K28CE	A30N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
K28CB	I41N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
K28CO	G29CO	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
K28CB	A42CO	-	-	-	-	X	-	-	-	-	-	-	-	1	L	7.5
K28CG	I41CO	-	-	-	-	-	-	-	-	-	-	X	-	1	L	8.0
K28NZ	A42CO	-	-	-	-	-	-	-	-	-	-	-	X	1	L	4.7
G29CA	A30CA	X	X	X	-	X	X	X	-	-	-	X	-	7	S	7.5
G29CO	A30CA	X	X	X	-	X	X	X	-	-	-	X	-	7	S	7.5
G29CA	A30CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
G29CO	A30CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
G29CO	I31CG2	X	-	-	-	-	-	X	-	-	-	-	-	2	M	8.5
G29CA	I41CA	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
G29CA	I41CB	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
G29CA	I41CD1	X	X	X	-	-	-	X	-	-	-	X	-	5	L	8.0
G29CO	I41CD1	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
G29CA	I41CG1	X	X	-	-	-	-	X	-	-	-	-	-	3	L	8.5
G29CO	I41CG1	X	-	-	-	-	-	X	-	-	-	-	-	2	L	8.5
G29CA	I41CG2	X	X	X	-	-	-	X	-	-	-	-	-	4	L	8.5
G29CA	I31CB	-	X	X	-	-	X	-	-	-	-	-	-	3	M	7.5
G29CO	I31CG1	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
G29CO	I41CG2	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
G29CO	A30CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
G29CO	I31CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
G29CA	I31CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
G29CO	I41CA	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
G29CO	I41CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
G29CA	A42CB	-	-	X	-	-	X	X	-	-	-	-	-	3	L	7.5
G29N	A30CA	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
G29CA	A30N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
G29CA	I41N	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
G29CA	I31CA	-	-	-	-	-	X	-	-	-	-	-	-	1	M	7.5
G29CA	A42CA	-	-	-	-	-	-	X	-	-	-	-	-	1	L	10.0
A30CA	I31CA	X	X	X	-	X	X	X	-	-	-	-	-	6	S	7.5
A30CB	I31CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
A30CA	I31CB	X	X	X	-	-	X	X	-	-	-	X	-	6	S	7.5
A30CA	I31CD1	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
A30CO	I31CD1	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
A30CA	I31CG1	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5

A30CO	I31CG1	X	X	X	-	X	X	X	-	-	-	-	-	6	S	7.5
A30CA	I31CG2	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
A30CO	I31CG2	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
A30CO	I31CA	-	X	X	-	X	X	X	-	-	-	-	-	5	S	7.5
A30CO	I31CB	-	X	X	-	X	X	-	-	-	-	-	-	4	S	7.5
A30CA	I31CO	-	-	X	-	-	X	-	-	-	-	X	-	3	S	7.5
A30CA	I32CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
A30CA	I31N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
A30CB	I31N	-	-	-	X	-	-	-	-	X	-	-	-	2	S	7.5
A30CO	I31N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
A30N	I32CG2	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
A30N	G33CA	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
A30N	V40CG1	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
A30CO	I31CO	-	-	-	-	X	-	X	-	-	-	-	-	2	S	7.5
A30CB	I31CO	-	-	-	-	-	-	X	-	-	-	-	-	1	S	10.0
I31CB	I32CB	X	X	X	-	-	-	-	-	-	-	X	-	4	S	8.0
I31CG1	V36CB	X	X	X	-	-	X	X	-	-	-	-	-	5	L	7.5
I31CB	V36CB	X	X	X	-	-	-	-	-	-	-	-	-	3	L	8.5
I31CO	I32CB	-	X	-	-	-	X	-	-	-	-	X	-	3	S	7.5
I31CO	I32CD1	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
I31CO	I32CG1	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
I31CG2	G33CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
I31CD1	V36CG2	-	X	X	-	-	-	-	-	-	-	-	-	2	L	8.5
I31CG2	V36CG2	-	X	-	-	-	-	X	-	-	-	-	-	2	L	8.5
I31CG1	I32CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
I31CO	I32CA	-	-	X	-	X	-	-	-	-	-	-	-	2	S	7.5
I31CD1	V36CB	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
I31CD1	V36CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
I31CA	V36CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
I31CB	V36CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
I31CG1	V36CG1	-	-	X	-	-	-	X	-	-	-	-	-	2	L	10.0
I31CA	V36CG2	-	-	X	-	-	-	X	-	-	-	-	-	2	L	10.0
I31CB	V39CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	L	10.0
I31N	I32CO	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
I31CB	I32N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
I31N	G33CO	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I31N	V40CG1	-	-	-	X	-	-	-	-	-	-	-	-	1	L	12.0
I31CG2	V36CB	-	-	-	-	-	X	-	-	-	-	-	-	1	L	7.5
I31CA	I32N	-	-	-	-	-	-	-	X	-	-	-	-	1	S	6.5
I32CG2	G33CA	X	-	X	-	-	X	X	-	-	-	-	-	4	S	7.5
I32CO	G33CA	X	X	X	-	X	X	X	-	-	-	X	-	7	S	7.5
I32CA	G33CA	-	X	-	-	X	X	X	-	-	-	-	-	4	S	7.5
I32CD1	G33CA	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
I32CB	G33CA	-	X	X	-	-	X	X	-	-	-	X	-	5	S	7.5
I32CG1	G33CA	-	-	X	-	-	-	-	-	-	-	X	-	2	S	8.0
I32CG2	L34CA	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
I32CG2	L34CD2	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
I32CG2	L34CO	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
I32CA	G33N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
I32N	L34CA	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CA	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CD1	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CG1	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CG2	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0

I32CO	L34N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CD1	M35N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
I32CA	G33CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
I32CB	G33CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
I32CG2	G33N	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
G33CA	L34CA	X	X	X	-	X	X	X	-	-	-	-	-	6	S	7.5
G33CA	L34CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
G33CA	L34CD1	X	-	-	-	-	-	X	-	-	-	-	-	2	S	8.5
G33CA	L34CD2	X	X	X	-	-	X	X	-	-	-	X	-	6	S	7.5
G33CA	L34CG	X	X	-	-	-	X	X	-	-	-	-	-	4	S	7.5
G33CA	L34CO	X	X	X	-	X	X	-	-	-	-	X	-	6	S	7.5
G33CA	V36CG1	X	X	X	-	-	-	X	-	-	-	-	-	4	M	8.5
G33CA	M35CG	X	X	-	-	-	-	-	-	-	-	-	-	2	M	8.5
G33CO	L34CA	-	X	X	-	X	X	-	-	-	-	-	-	4	S	7.5
G33CA	M35CB	-	X	X	-	-	-	-	-	-	-	-	-	2	M	8.5
G33CA	V36CB	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
G33CO	V36CG1	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
G33CA	V36CG2	-	X	X	-	-	X	-	-	-	-	-	-	3	M	7.5
G33CA	M35CO	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
G33N	M35CB	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
G33CA	M35N	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
G33CO	L34CO	-	-	-	-	X	-	X	-	-	-	-	-	2	S	7.5
G33CO	V36CA	-	-	-	-	X	-	-	-	-	-	-	-	1	M	7.5
G33CO	L34CB	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
G33CO	L34CD2	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
G33CO	L34CG	-	-	-	-	-	X	X	-	-	-	-	-	2	S	7.5
G33CO	V36CG2	-	-	-	-	-	-	X	-	-	-	-	-	1	M	10.0
G33N	L34CG	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
G33CA	V36CA	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
L34CG	M35CB	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
L34CA	M35CA	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
L34CO	M35CA	X	X	-	-	X	X	-	-	-	-	X	-	5	S	7.5
L34CA	M35CB	X	X	X	-	-	X	-	-	-	-	-	-	4	S	7.5
L34CB	M35CB	X	X	X	-	-	X	-	-	-	-	-	-	4	S	7.5
L34CO	M35CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
L34CB	M35CE	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
L34CA	M35CG	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
L34CO	M35CG	X	X	X	-	-	X	-	-	-	-	X	-	5	S	7.5
L34CD1	M35CA	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
L34CD2	M35CB	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
L34CD1	M35CB	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
L34CD2	M35CA	-	-	X	-	X	-	-	-	-	-	X	-	3	S	7.5
L34CG	M35CA	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
L34CG	M35CG	-	-	X	-	-	-	X	-	-	-	-	-	2	S	10.0
L34CG	M35CE	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
L34CA	V36CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
L34CO	V36CG1	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
L34N	M35CA	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
L34N	M35CG	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
L34N	M35CO	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
L34CB	M35N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
L34N	V36CG1	-	-	-	X	-	-	-	X	X	-	-	-	3	M	6.5
L34N	V36CG2	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
L34CO	M35CO	-	-	-	-	X	-	X	-	-	-	X	-	3	S	7.5

L34CA	M35CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L34CB	M35CA	-	-	-	-	-	X	X	-	-	-	X	-	3	S	7.5
L34CB	M35CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
L34CO	V36CA	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
L34CO	V36CB	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
M35CG	V36CA	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
M35CA	V36CG1	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
M35CA	V36CA	-	X	X	-	X	X	X	-	-	-	-	-	5	S	7.5
M35CB	V36CA	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
M35CG	V36CB	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
M35CB	V36CG1	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
M35CG	V36CG1	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
M35CB	V36CG2	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
M35CB	G37CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
M35CG	G37CA	-	X	-	-	-	-	-	-	-	-	-	-	1	M	8.5
M35CO	V36CA	-	-	X	-	-	-	-	-	-	-	X	-	2	S	8.0
M35CA	V36CG2	-	-	X	-	-	X	X	-	-	-	-	-	3	S	7.5
M35N	V36CG2	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
M35CG	V36CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
M35CO	V36CG1	-	-	-	-	-	X	X	-	-	-	-	-	2	S	7.5
M35CG	V36CG2	-	-	-	-	-	-	X	-	-	-	-	-	1	S	10.0
M35CO	V36CG2	-	-	-	-	-	-	X	-	-	-	-	-	1	S	10.0
V36CB	G37CA	X	-	X	-	-	X	X	-	-	-	-	-	4	S	7.5
V36CO	G37CA	X	-	-	-	-	-	X	-	-	-	-	-	2	S	8.5
V36CG2	G37CO	-	X	X	-	-	X	-	-	-	-	-	-	3	S	7.5
V36CB	G37CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
V36CG1	G37CO	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
V36CA	G37N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V36CG2	G37N	-	-	-	X	-	-	-	X	X	-	-	-	3	S	6.5
V36CO	G37CO	-	-	-	-	X	-	-	-	-	-	-	-	1	S	7.5
V36CG1	G37CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
V36CA	G37CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
V36CG1	V39CB	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
G37CA	G38CA	X	X	X	-	-	-	-	-	-	-	-	-	3	S	8.5
G37N	V39CB	-	-	-	X	-	-	-	-	-	-	-	-	1	M	12.0
G37N	V39CG1	-	-	-	-	-	-	-	-	X	-	-	-	1	M	7.5
G37CA	V39CB	-	-	-	-	-	-	-	-	-	-	X	-	1	M	8.0
V39CB	I41CB	X	-	-	-	-	-	-	-	-	-	-	-	1	M	8.5
V40CG2	I41CB	X	X	-	-	-	X	X	-	-	-	-	-	4	S	7.5
V40CA	I41CB	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
V40CA	I41CG1	X	X	X	-	-	X	X	-	-	-	-	-	5	S	7.5
V40CA	I41CA	-	X	X	-	-	X	X	-	-	-	-	-	4	S	7.5
V40CB	I41CB	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
V40CB	I41CG1	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
V40CB	I41CD1	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
V40CG2	I41CD1	-	X	-	-	-	-	-	-	-	-	-	-	1	S	8.5
V40CG2	I41CG1	-	-	X	-	-	-	X	-	-	-	-	-	2	S	10.0
V40CO	I41CB	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
V40CA	I41CD1	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
V40CA	I41CG2	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
V40CB	I41CG2	-	-	X	-	-	-	X	-	-	-	-	-	2	S	10.0
V40CG2	I41CG2	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
V40CO	A42CO	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0
V40CO	A42CB	-	-	X	-	-	-	-	-	-	-	-	-	1	M	10.0

V40N	I41CA	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V40N	I41CB	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V40N	I41CD1	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V40CA	I41N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V40CO	I41N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
V40CG2	I41CA	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
V40CG2	I41N	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
V40CG2	A42CA	-	-	-	-	-	-	-	-	-	X	-	-	1	M	7.5
V40CB	I41CO	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0
I41CG1	A42CA	X	X	X	-	-	-	X	-	-	-	X	-	5	S	8.0
I41CA	A42CA	-	X	X	-	-	X	X	-	-	-	-	-	4	S	7.5
I41CB	A42CA	-	X	X	-	-	X	-	-	-	-	X	-	4	S	7.5
I41CD1	A42CA	-	X	X	-	-	-	-	-	-	-	-	-	2	S	8.5
I41CG2	A42CA	-	X	X	-	-	X	-	-	-	-	-	-	3	S	7.5
I41CG2	A42CO	-	-	X	-	-	X	-	-	-	-	-	-	2	S	7.5
I41CO	A42CO	-	-	X	-	-	-	X	-	-	-	-	-	2	S	10.0
I41CB	A42CB	-	-	X	-	-	-	-	-	-	-	-	-	1	S	10.0
I41N	A42CA	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
I41CA	A42N	-	-	-	X	-	-	-	-	-	-	-	-	1	S	12.0
I41CA	A42CB	-	-	-	-	X	-	X	-	-	-	-	-	2	S	7.5
I41CA	A42CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
I41CB	A42CO	-	-	-	-	-	X	-	-	-	-	-	-	1	S	7.5
I41CG2	A42N	-	-	-	-	-	-	-	X	X	-	-	-	2	S	6.5
I41CO	A42CA	-	-	-	-	-	-	-	-	-	-	X	-	1	S	8.0

SUMMARY:

SEQUENTIAL CONTACTS:	264
MEDIUM RANGE CONTACTS:	93
LONG RANGE CONTACTS:	104
INTERMOLECULAR CONTACTS:	26
TOTAL w/o INTRARES.:	487