Supporting Information

Supramolecular Protein Structure Determination by Site-Specific Long-Range Intermolecular Solid State NMR Spectroscopy

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Materials and Methods

Sample Preparation

Samples of GB1 were prepared by bacterial overexpression in two batches: (a) ^{15}N isotopically labeled in media containing ^{15}N ammonium chloride and natural abundance glucose, and (b) ^{13}C isotopically labeled in 1,3-^{13}C-glycerol and natural abundance sodium carbonate and ammonium chloride. The sample was prepared by physically mixing a 50:50 ratio of these two preparations prior to nanocrystalline precipitation by previously reported methods. Additional samples of ^{13}C and ^{15}N enriched GB1 were also prepared in media containing ^{15}N ammonium chloride and either 2-^{13}C-glycerol and calcium ^{13}C-carbonate as reported earlier.[1] Samples (each with ~18 mg protein) were packed into the central 80% of limited speed 3.2 mm Varian rotors (Varian, Inc., Fort Collins, Colorado).

Solid-state NMR spectroscopy

Experiments were performed using a 500 MHz InfinityPlus spectrometer (Varian, Inc., Palo Alto, California and Fort Collins, Colorado) equipped with a 3.2 mm T3 Balun™ ^{1}H-^{13}C-^{15}N MAS probe. Pulse widths ($\pi/2$) for ^{1}H, ^{13}C, and ^{15}N were 2.55 μs, 2.9 μs, and 5.5 μs respectively. Spinning was controlled with a Varian MAS controller to 11,111 ± 2 Hz. TPPM decopuling (~75 kHz, ^{1}H pulse width 6.6 μs, total phase difference 15°) was used during acquisition and ^{15}N evolution. TPPM during REDOR periods was independently optimized at a higher power level (~100 kHz, 5 μs, 11°).

ZF-TEDOR 2D planes with 8.64, 16.86 and 21.6 ms of mixing were acquired. Each was digitized to 3072 x 10 μs in the direct (^{13}C) and 80 x 180 μs in the indirect (^{15}N) dimension. Total measurement times were 21.7, 34.6 and 26 hrs.

Structure Calculations

Intermolecular TEDOR restraints were extracted from 2D TEDOR planes by first picking peaks from the longest (21.6 ms) ^{15}N-^{13}C mixing experiments and then determining which of these peaks also appeared in the shorter mixing experiments (Figure S1). A small subset of peaks—which we attribute to natural abundance ^{13}C sites on the ^{15}N labeled sample—appear at the shortest mixing time; however, these did not prove difficult to differentiate from the labeled sites. Specifically, the maximum ^{13}C-^{15}N transfer for TEDOR is theoretically 52%, and we observe on the order of 40% for 1-bond (1.45 Å, at 1.44 ms) and 30% for a 2-bond (2.45 Å, at 5.76 ms) ^{15}N-^{13}C distances. Thus the strongest natural abundance peaks will appear at 0.4% and 0.3% respectively of the reference spectrum, and these intensities decay at longer mixing times. For example, the natural abundance peaks observed (Figure S1a, labeled with asterisks) decay below the noise threshold at longer mixing times (Figure S1b and Figure 1). At mixing times of ~20 ms, the natural abundance ^{13}C sites decay to a small fraction of their initial intensity, and the intermolecular correlations increase in intensity.

Intermolecular TEDOR restraints were assumed to have distance ranges <5 Å for restraints first appearing at 8.64 ms mixing, <7 Å for peaks that were first observed in the 16.86 ms data and <8 Å for those peaks only seen in the 21.6 ms mixing time spectrum. These distances correspond to the longest-range correlations observed in the undiluted ^{15}N-^{13}C sample[2] at moderate (~8 ms, 6 Å) and long (~15 ms, 8 Å) mixing times, corrected for the relative amount of sample and signal averaging time; i.e., with 25% of the sample quantity (50% is labeled with either ^{15}N or ^{13}C, and only 50% of intermolecular interfaces have the complementary labeling to enable ^{15}N-^{13}C correlations) but twice the signal

averaging time, we observed a ~2-fold decrease in signal to noise. Therefore we adjusted the distance threshold (assuming the linear rate regime of TEDOR buildup) by 2^(-1/3) = ~0.8.

Correlations were assigned in a manner explicitly taking ambiguity into account; possible assignments included any ^{15}N resonance within 0.25 ppm and any ^{13}C resonance within 0.15 ppm of the observed crosspeak (corresponding to half the average linewidths in each dimension). This procedure resulted in restraints with up to four-fold ambiguity in each dimension. For example, the peak at 123.3 ppm ^{15}N, and 173.1 ppm ^{13}C (Figures 1, S1) has nine possible assignments (three-fold degenerate in each dimension): Y3N, K13N or D47N correlated to K4C, G9C or T11C. However, 20 restraints were completely unambiguous, while 18 were two-fold and 14 were threefold degenerate. The remaining 36 were four or more fold degenerate (see Table S1).

Figure S3 and S4 illustrate the results for the trigonal and orthorhombic crystal packing geometries. From these refined structures each restraint could be unambiguously assigned to one possible ^{15}N-^{13}C pair within 8 Å, for the example above a β3-β2' correlation D47-T11C. Some of these assigned restraint lists are shown in Figure S5 and they are all listed the last column of Table S1. Despite these assignments, ambiguous restraint lists were used for all structure calculations and can be found in the BMRB listing for this structure, 16836.

The crystal lattices used as the starting structures for the trigonal[3] (2QMT) and orthorhombic[4] (2GI9) calculations were generated using SwissPDB viewer[5] (http://www.expasy.org/spdbv/) selecting all GB1 monomers with ^{15}N sites within 8 Å of a ^{13}C site on the central monomer. In both cases a total of six GB1 molecules were found

to have ^{15}N-^{13}C pairs less than 8 Å apart. In the case of the trigonal packing one of those monomers was only restrained by one correlation, and as such did not converge to a unique conformation in the final calculations. Thus in Figures S3 and S6 only the five well-restrained monomers are shown. Similarly for the orthorhombic lattice the sixth monomer was not restrained at all and is not shown in Figures S4 and S6. Therefore, for the *de novo* annealing calculation five copies of the lowest energy model from the intramolecular TEDOR structure[2] (2KQ4) were manually translated and rotated into a grid with four monomers in plane and one above them out of plane. VMD-XPLOR[6] (http://vmd-xplor.cit.nih.gov/) was used to create the initial conditions for the *in silico* annealing. All monomers were ~20 Å apart, and positioned in a rough array around the central GB1, corresponding to the four areas of intermolecular contact observed. The calculations proved to be relatively insensitive to starting conditions, converging to a similar structure from multiple starting orientations, with the only requirement being all monomers must be separated by an equal distance from the central monomer.

Simulated annealing calculations were performed using the python extension of XPLOR-NIH.[7] Intermolecular TEDOR restraints were applied ambiguously from the central GB1 molecule to any other GB1, enforcing the intermolecular nature of the data. Intramolecular restraints were applied to each monomer and included TEDOR distances and TALOS dihedral angle restraints. A symmetry potential was used to enforce similarity between all monomers in each calculation, as required by our NMR data which shows only a single set of peaks for each residue. For the docking procedure this potential was also used to fix the internal coordinates of the monomers: by fixing the atom positions of the central monomer and applying a large symmetry potential the center of

mass and orientation of the peripheral GB1 monomers were allowed to change while keeping the internal structure fixed. High temperature dynamic times of 20 ps were used for the trigonal and *in silico* calculations and 40 ps for the orthorhombic to trigonal annealing followed by annealing times of 60 ps. In all cases 600 structures were calculated with the set of lowest 10 energy structures reported. bbRMSDs reported for these sets are the average of the 10 RMSDs for the backbone aligned in VMD-XPLOR, reported error is the standard deviation. In the cases where bbRMSDs are reported to crystal structures the same structures are aligned to the X-ray crystal lattice in VMD-XPLOR and the RMSD of all 10 structures, to the X-ray was reported.

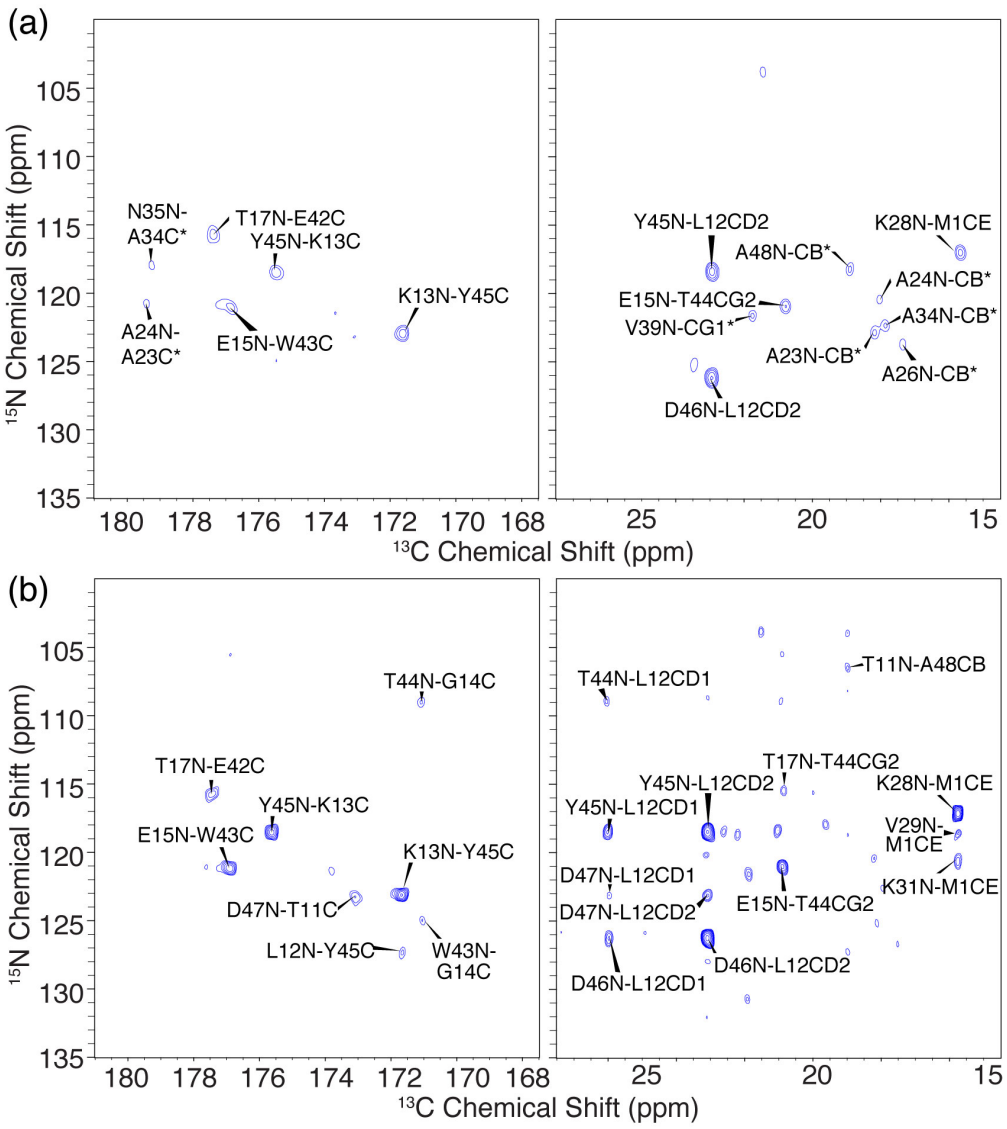

Figure S1. 2D ^{13}C-^{15}N planes from the 3D ZF-TEDOR spectrum collected with 50% U-^{15}N GB1 physically mixed with 50% 1,3-^{13}C glycerol labeled GB1. TEDOR mixing times of (a) 8.64 ms and (b) 16.48 ms are shown. Spectra were acquired at 500 MHz (^{1}H) with 21.6 ms ^{15}N-^{13}C mixing, 14.4 ms t_{1max} (^{15}N evolution) and 30.7 ms ^{13}C acquisition time. Total measurement time was (a) 21.7 and (b) 34.6 hours. Peaks in (a) labeled with asterisks are attributed to natural abundance ^{13}C in the ^{15}N labeled samples. These weak peaks decrease in intensity at longer than 8 ms mixing times and therefore are concluded to be intramolecular and were not included in the restraint lists for the structure calculations.

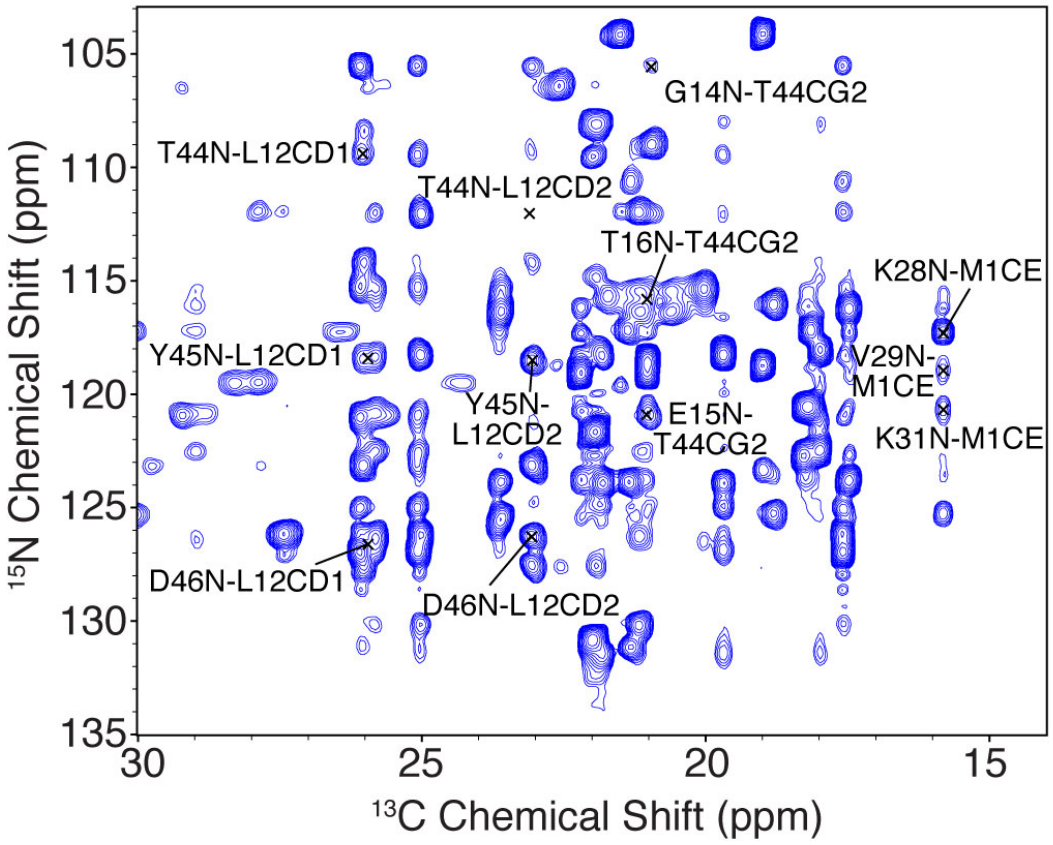

Figure S2. 2D TEDOR correlation spectrum of 1,3-^{13}C glycerol, ^{15}N labeled GB1 with 14.4 ms mixing time. Data were acquired with 28.8 ms t_{1max} (^{15}N evolution) and 46.1 ms ^{13}C acquisition at 500 MHz ^{1}H frequency with a 11,111 Hz MAS rate and a total measurement time of 40.5 hours. This spectrum is the longest mixing undiluted TEDOR experiment reported earlier.[2] In addition to strong intramolecular peaks, correlations which also appear in the intermolecular TEDOR can be attributed to intermolecular contacts and are labeled with X's. In some cases, the intermolecular peak was obscured by strong intramolecular peaks, in which case the X is used to illustrate peaks that were impossible to observe in the uniformly labeled data.

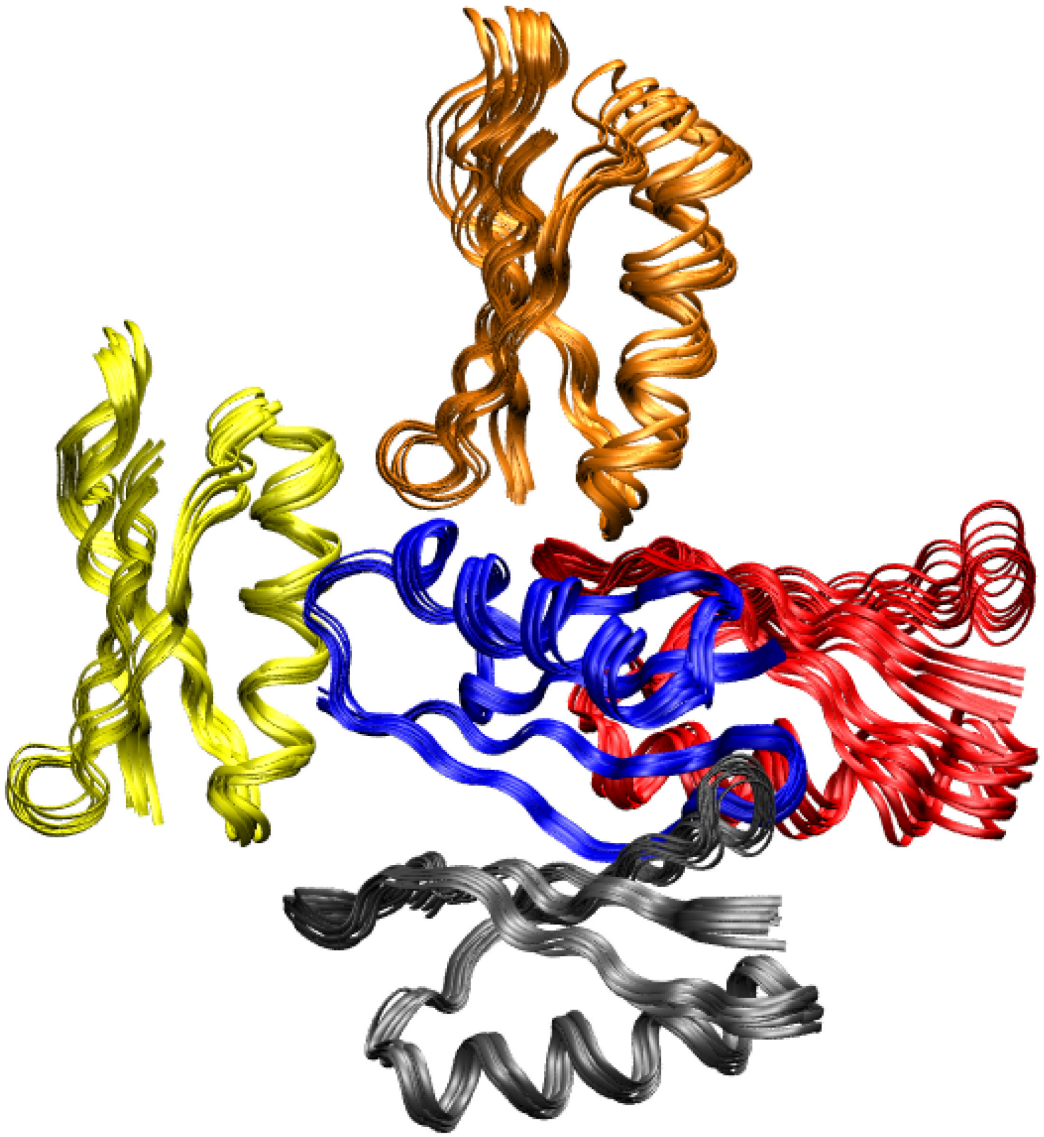

Figure S3. Quaternary structure of GB1 (10 lowest energy structures out of 600) as determined by simulated annealing structure calculations initiated from the trigonal crystal lattice (PDB ID 2QMT). Ambiguous intermolecular TEDOR restraints were used for which all possible ^{15}N and ^{13}C assignments for a given correlation were included. One monomer was poorly restrained in the calculation, with only one correlation in the intermolecular TEDOR data, and is not shown. Backbone RMSD is 0.8 ± 0.3 Å for the 5 monomers shown here.

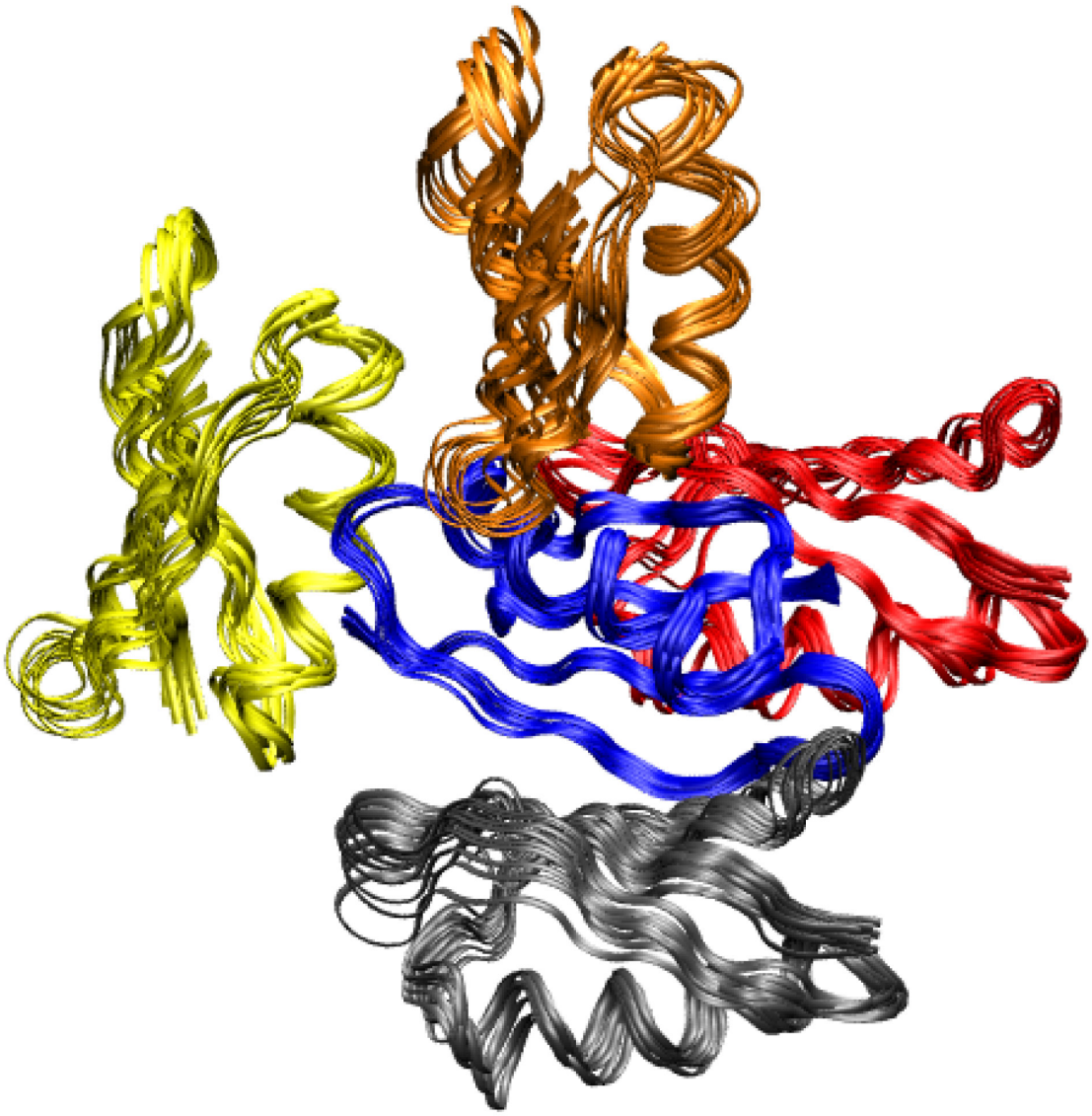

Figure S4. Quaternary structure of GB1 (10 lowest energy structures out of 600) as determined by simulated annealing structure calculations initiated from the orthorhombic crystal lattice (PDB ID 2GI9). Ambiguous intermolecular TEDOR restraints were used for which all possible ^{15}N and ^{13}C assignments for a given correlation were included. One monomer was not restrained in the calculation, and is not shown. Backbone RMSD is 1.4 ± 0.4 Å for the 5 monomers shown here.

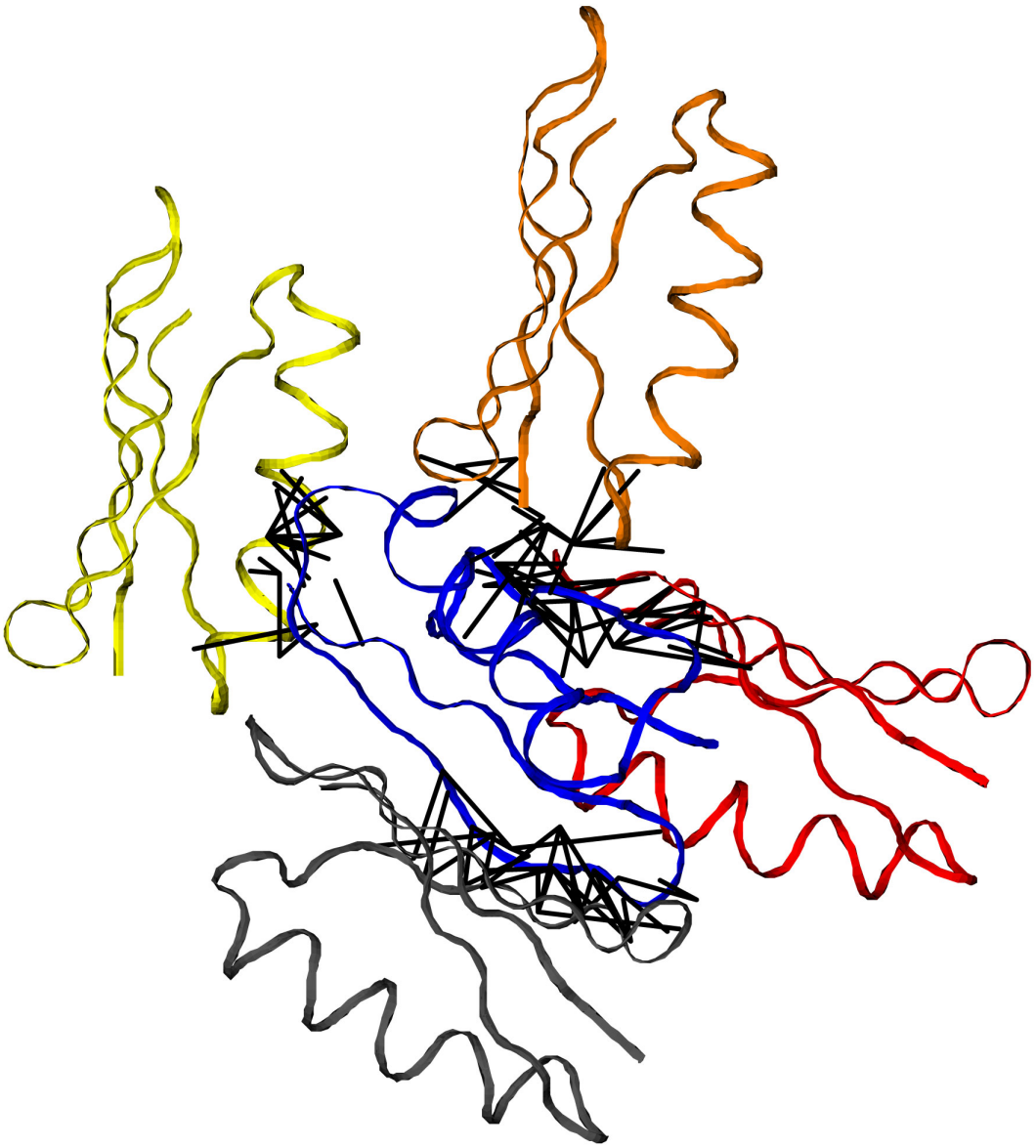

Figure S5. Intermolecular TEDOR restraints used in XPLOR-NIH calculations. Restraints are shown in black on the lowest energy structure initated with the trigonal lattice (Figure S3). All restraints are derived from TEDOR experiments on a sample of 50% U-^{15}N GB1 physically mixed with 50% 1,3-^{13}C glycerol labeled GB1 (Figure 1, Figure S1).

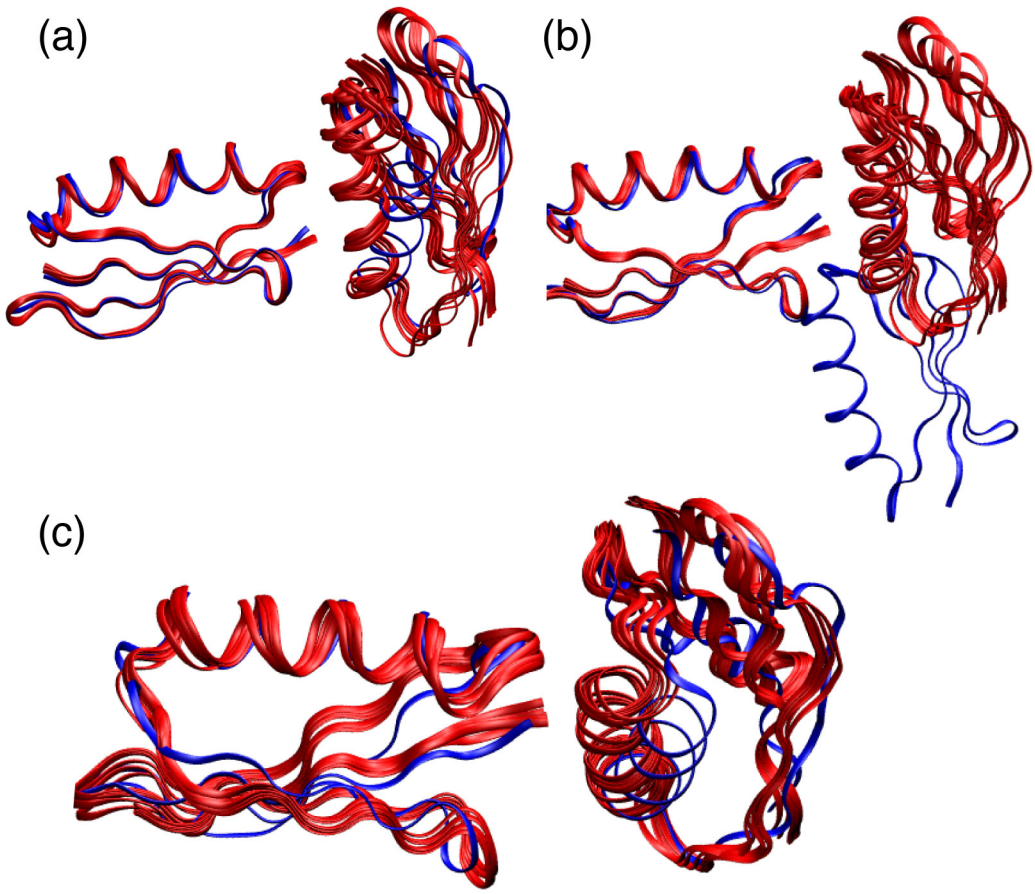

Figure S6. Two monomers (10 lowest energy out of 600 calculated) taken from the trigonal calculation with intermolecular TEDOR restraint lists. These two monomers (red) aligned by the central monomer overlaid with (a) the trigonal (2QMT, blue) and (b) the orthorhombic (2GI9, blue) X-ray crystal lattices. Backbone RMSDs for the central monomers are (a) 0.73 ± 0.04 Å and (b) 0.73 ± 0.04 Å. Backbone RMSDs for both monomers shown are (a) 4.1 ± 0.4 Å and (b) 13.6 Å ± 0.3 Å. When aligned by both monomers to the trigonal crystal structure (c) the backbone RMSD is 2.7 ± 0.3 Å.

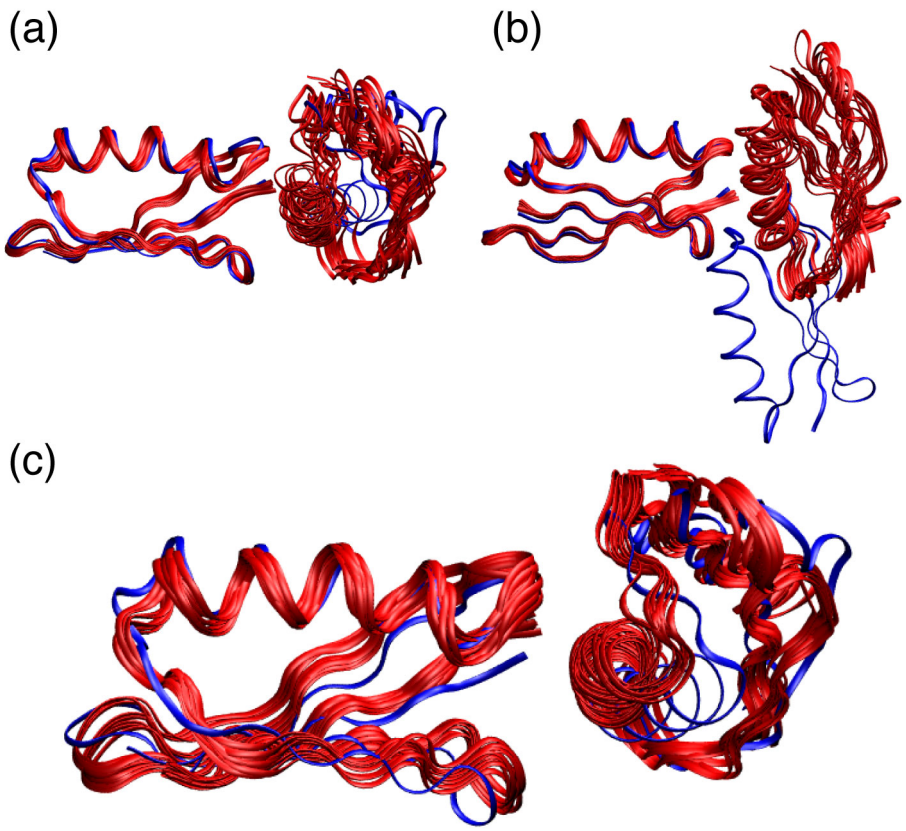

Figure S7. Two monomers (10 lowest energy out of 600 calculated) taken from the orthorhombic calculation with intermolecular TEDOR restraint lists. These two monomers (red) aligned by the central monomer overlaid with (a) the trigonal (2QMT, blue) and (b) the orthorhombic (2GI9, blue) X-ray crystal lattices. Backbone RMSDs for the central monomers are (a) 1.00 ± 0.07 Å and (b) 0.94 ± 0.07 Å. Backbone RMSDs for both monomers shown are (a) 4.7 ± 0.4 Å and (b) 15.8 Å ± 0.7 Å. When aligned by both monomers to the trigonal crystal structure (c) the backbone RMSD is 2.8 ± 0.3 Å.

Table S1. Intermolecular TEDOR Restraints.

Residue/Atom	Residue/Atom	Distance (Å)	Degeneracy	Manual Assignment
1CE	31N	5	1	K31N-M1CE
31N	1CE	5	1	K31N-M1CE
20CB	31NZ	8	1	K31NZ-A20CB
31NZ	20CB	8	1	K31NZ-A20CB
1CB	31NZ	5	1	K31NZ-M1CB
31NZ	1CB	5	1	K31NZ-M1CB
1CE	31NZ	5	1	K31NZ-M1CE
31NZ	1CE	5	1	K31NZ-M1CE
21CG1	31NZ	5	1	K31NZ-V21CG1
31NZ	21CG1	5	1	K31NZ-V21CG1
12N	48CB	5	1	L12N-A48CB
48CB	12N	5	1	L12N-A48CB
1N	27CG	7	1	M1N-A27CG
27CG	1N	7	1	M1N-A27CG
1N	27CD	5	1	M1N-E27CD
27CD	1N	5	1	M1N-E27CD
11N	48CB	8	1	T11N-A48CB
48CB	11N	8	1	T11N-A48CB
12CD2	44N	7	1	T44N-L12CD2
44N	12CD2	7	1	T44N-L12CD2
20N	31CG or 31CG	7	2	A20N-K31CG
31CG or 6CG1	20N	7	2	A20N-K31CG
46N or 6N	12CD2	5	2	D46N-L12CD2
12CD2	46N or 6N	5	2	D46N-L12CD2
14N	44CG2 or 29CG1	5	2	G14N-T44CG2
44CG2 or 29CG1	14N	5	2	G14N-T44CG2
14N	43C or 26C	5	2	G14N-W43C
43C or 26C	14N	5	2	G14N-W43C
1CE	28N or 25N	5	2	K28N-M1CE
28N or 25N	1CE	5	2	K28N-M1CE
12N	45C or 16C	5	2	L12N-Y45C
45C or 16C	12N	5	2	L12N-Y45C
1N	24CB or 23CB	8	2	M1N-A24CB
24CB or 23CB	1N	8	2	M1N-A24CB
12CD2	53N or 51N	7	2	T53N-L12CD2
53N or 51N	12CD2	7	2	T53N-L12CD2
15C	43N or 8N	8	2	W43N-E15C
43N or 8N	15C	8	2	W43N-E15C
46N	12CD1 or 7CD1 or 13CG	5	3	D46N-L12CD1
12CD2	47N or 3N or 13N	5	3	D47N-L12CD2
47N or 3N or 13N	12CD2	5	3	D47N-L12CD2
31NZ	20C or 42C or 32C	7	3	K31NZ-A20C
20C or 42C or 32C	31NZ	7	3	K31NZ-A20C
44N	14C or 18C or 1C	5	3	T44N-G14C

Residue/Atom	Residue/Atom	Distance (Å)	Degeneracy	Manual Assignment
14C or 18C or 1C	44N	5	3	T44N-G14C
44N	7CD1 or 13CG or 12CD1	5	3	T44N-L12CD1
12CD1 or 7CD1 or 13CG	44N	5	3	T44N-L12CD1
12CD2	45N or 30N or 54N	5	3	Y45N-L12CD2
45N or 30N or 54N	12CD2	5	3	Y45N-L12CD2
11CG2	45N or 30N or 54N	7	3	Y45N-T11CG2
11CG2	45N or 30N or 54N	7	3	Y45N-T11CG2
45N or 30N or 54N	11CG2	7	3	Y45N-T11CG2
1CE	42N or 45N or 48N or 30N	7	4	F30N-M1CE
45N or 30N or 42N or 48N	1CE	7	4	F30N-M1CE
13N or 47N	45C or 16C	5	4	K13N-Y45C
45C or 16C	13N or 47N	5	4	K13N-Y45C
31NZ	21C or 3C or 40C or 2C	5	4	K31NZ-V21C
21C or 3C or 2C or 40C	31NZ	5	4	K31NZ-V21C
19N or 2N	24CB or 23CB	7	4	Q2N-A23CB
24CB or 23CB	2N or 19N	8	4	Q2N-A23CB
46N or 6N	12CD1 or 7CD1 or 13CG	5	6	D46N-L12CD1
12CD1 or 7CD1 or 13CG	46N or 6N	5	6	D46N-L12CD1
36CB or 8CB	32NE2 or 17N or 22N	7	6	Q32NE2-D36CB
32NE2 or 17N or 22N	36CB or 8CB	7	6	Q32NE2-D36CB
44CG2 or 29CG1	16N or 22N or 32NE2	7	6	T16N-T44CG2
16N or 22N or 32NE2	44CG2 or 29CG1	7	6	T16N-T44CG2
43N or 8N	14C or 18C or 1C	5	6	W43N-G14C
14C or 18C or 1C	43N or 8N	5	6	W43N-G14C
46N or 6N	12CA or 47CA or 24CA or 23CA	5	8	D46N-L12CA
12CA or 47CA or 24CA or 23CA	46N or 6N	5	8	D46N-L12CA
44CG2 or 29CG1	15N or 32N or 36N or 10N	5	8	E15N-T44CG2
15N or 32N or 36N or 10N	44CG2 or 29CG1	5	8	E15N-T44CG2
43C or 26C	15N or 32N or 36N or 10N	5	8	E15N-W43C
15N or 32N or 36N or 10N	43C or 26C	5	8	E15N-W43C
12CD1 or 7CD1 or 13CG	47N or 3N or 13N	7	9	D47N-L12CD1
47N or 3N or 13N	12CD1 or 7CD1 or 13CG	7	9	D47N-L12CD1
11C or 9C or 4C	47N or 3N or 13N	5	9	D47N-T11C
47N or 3N or 13N	9C or 4C or 11C	5	9	D47N-T11C
12CD1 or 7CD1 or 13CG	45N or 30N or 54N	5	9	Y45N-L12CD1
45N or 30N or 54N	7CD1 or 13CGor 12CD1	5	9	Y45N-L12CD1
47N or 3N or 13N	12CA or 47CA or 24CA or 23CA	5	12	D47N-L12CA
12CA or 47CA or 24CA or 23CA	47N or 3N or 13N	5	12	D47N-L12CA

Residue/Atom	Residue/Atom	Distance (Å)	Degeneracy	Manual Assignment
14C or 18C or 1C	42N or 45N or 48N or 30N	8	12	E42N-G14C
45N or 30N or 42N or 48N	14C or 18C or 1C	8	12	E42N-G14C
19C or 25C or 13C or 49C or 52C	45N or 30N or 54N	5	15	Y45N-K13C
45N or 30N or 54N	19C or 25C or 13C or 49C or 52C	5	15	Y45N-K13C
12CA or 47CA or 24CA or 23CA	45N or 30N or 42Nor 48N	5	16	A48N-L12CA
45N or 30N or 42N or 48N	12CA or 47CA or 24CAor 23CA	5	16	A48N-L12CA

Table S2. Intramolecular TEDOR Distance Restraints

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
1	N	1	CA	1.48	0.10	M1N-CA
1	N	1	CB	2.44	0.10	M1N-CB
1	N	1	CE	3.77	0.60	M1N-CE
1	N	1	CG	3.61	0.50	M1N-CG
1	N	1	CB	2.44	0.10	M1N-CB
1	N	1	CG	3.74	0.20	M1N-CG
1	N	3	CG	6.34	3.28	M1N-Y3CG
1	N	19	CD	4.14	0.24	M1N-E19CD
1	N	20	CB	6.16	3.33	M1N-A20CB
1	N	20	CA	5.20	4.20	M1N-A20CA
2	N	1	CB	3.32	0.10	Q2N-M1CB
2	N	1	CE	4.20	1.04	Q2N-M1CE
2	N	1	CG	3.01	0.10	Q2N-M1CG
2	N	1	CB	3.34	0.23	Q2N-M1CB
2	N	1	CE	4.06	3.06	Q2N-M1CE
2	N	1	CG	2.86	0.10	Q2N-M1CG
2	N	2	CA	1.44	0.10	Q2N-CA
2	NE2	2	CD	1.82	0.82	Q2NE2-CD
2	N	2	CG	3.12	0.10	Q2N-CG
2	NE2	2	CG	2.78	0.10	Q2NE2-CG
2	N	2	CD	5.18	0.82	Q2N-CD
2	NE2	2	CD	1.75	0.75	Q2NE2-CD
2	N	3	CA	4.13	1.02	Q2N-Y3CA
2	N	3	CG	4.65	0.48	Q2N-Y3CG
2	NE2	17	CG2	4.96	0.10	Q2NE2-T17CG2
2	NE2	19	CD	5.53	0.25	Q2NE2-E19CD
3	N	1	CE	5.42	1.45	Y3N-M1CE
3	N	1	CG	4.82	1.41	Y3N-M1CG
3	N	2	CA	2.55	0.11	Y3N-Q2CA
3	N	2	CA	2.33	0.10	Y3N-Q2CA
3	N	3	CA	1.44	0.10	Y3N-CA
3	N	3	CG	3.07	0.34	Y3N-CG
3	N	18	CG2	4.77	0.35	Y3N-T18CG2
3	N	19	CD	7.08	0.35	Y3N-E19CD
4	N	3	CA	2.57	0.19	K4N-Y3CA
4	N	3	CG	4.15	0.27	K4N-Y3CG
4	N	4	CA	1.43	0.10	K4N-CA
4	N	4	CB	2.43	0.21	K4N-CB
4	N	4	CD	4.87	0.10	K4N-CD
4	NZ	4	CD	2.95	1.95	K4NZ-CD
4	N	4	CG	3.94	0.10	K4N-CG
4	N	4	CA	1.44	0.10	K4N-CA
4	N	4	CB	2.42	0.10	K4N-CB
4	NZ	4	CD	3.25	1.10	K4NZ-CD

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
4	N	4	CG	3.10	1.10	K4N-CG
4	NZ	6	CD1	4.60	0.15	K4NZ-I6CD1
4	NZ	6	CG2	7.30	5.73	K4NZ-I6CG2
4	N	6	CD1	6.89	1.83	K4N-I6CD1
4	NZ	6	CD1	5.05	0.44	K4NZ-I6CD1
4	NZ	15	CD	3.71	0.10	K4NZ-E15CD
4	NZ	17	CG2	6.12	0.10	K4NZ-T17CG2
4	N	17	CG2	4.90	3.90	K4N-T17CG2
4	N	51	CG2	5.15	0.40	K4N-T51CG2
4	N	51	CG2	5.58	0.51	K4N-T51CG2
4	NZ	51	CG2	6.40	1.66	K4NZ-T51CG2
4	N	52	CG	6.05	1.49	K4N-F52CG
5	N	4	CB	3.50	0.44	L5N-K4CB
5	N	4	CD	5.11	0.10	L5N-K4CD
5	N	4	CG	3.43	0.10	L5N-K4CG
5	N	4	CA	2.54	0.10	L5N-K4CA
5	N	4	CB	3.34	0.12	L5N-K4CB
5	N	4	CD	5.25	4.25	L5N-K4CD
5	N	5	CA	1.42	0.10	L5N-CA
5	N	5	CG	3.05	1.10	L5N-CG
5	N	16	CG2	4.83	0.98	L5N-T16CG2
5	N	16	CG2	5.18	1.26	L5N-T16CG2
5	N	17	CG2	5.46	0.10	L5N-T17CG2
5	N	18	CG2	6.15	1.88	L5N-T18CG2
5	N	30	CG	5.68	0.62	L5N-F30CG
6	N	5	CD2	3.29	0.10	I6N-L5CD2
6	N	5	CD2	3.19	2.19	I6N-L5CD2
6	N	6	CA	1.44	0.10	I6N-CA
6	N	6	CB	2.61	0.10	I6N-CB
6	N	6	CD1	3.39	0.10	I6N-CD1
6	N	6	CG1	2.76	0.10	I6N-CG1
6	N	6	CG2	3.30	1.10	I6N-CG2
6	N	6	CB	2.50	0.32	I6N-CB
6	N	6	CD1	3.62	0.33	I6N-CD1
6	N	6	CG2	3.97	0.30	I6N-CG2
6	N	15	CD	5.76	0.10	I6N-E15CD
6	N	53	CG2	3.54	1.10	I6N-T53CG2
6	N	53	CG2	3.39	1.10	I6N-T53CG2
6	N	54	CG1	5.89	2.02	I6N-V54CG1
7	N	6	CA	2.21	0.10	L7N-I6CA
7	N	6	CD1	4.74	3.74	L7N-I6CD1
7	N	6	CG1	4.35	0.27	L7N-I6CG1
7	N	6	CG2	3.04	0.10	L7N-I6CG2
7	N	6	CB	3.50	0.10	L7N-I6CB
7	N	6	CD1	4.55	3.55	L7N-I6CD1
7	N	6	CG2	3.54	0.10	L7N-I6CG2

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
7	N	7	CA	1.45	0.12	L7N-CA
7	N	7	CD1	3.28	0.10	L7N-CD1
7	N	7	CD2	3.50	1.10	L7N-CD2
7	N	7	CB	2.45	0.34	L7N-CB
7	N	7	CD1	3.48	1.10	L7N-CD1
7	N	7	CD2	3.53	1.12	L7N-CD2
7	N	15	CD	5.62	0.10	L7N-E15CD
7	N	54	CG1	4.87	0.70	L7N-V54CG1
8	N	6	CG2	4.67	0.24	N8N-I6CG2
8	ND2	6	CG2	5.57	1.65	N8ND2-I6CG2
8	N	6	CD1	7.30	3.14	N8N-I6CD1
8	N	7	CA	2.56	0.10	N8N-L7CA
8	N	7	CD1	4.79	3.79	N8N-L7CD1
8	N	7	CD2	4.61	1.10	N8N-L7CD2
8	N	7	CB	3.67	0.20	N8N-L7CB
8	N	8	CA	1.50	0.10	N8N-CA
8	N	8	CB	2.21	0.10	N8N-CB
8	ND2	8	CB	2.71	0.47	N8ND2-CB
8	ND2	8	CG	1.41	0.10	N8ND2-CG
8	N	8	CA	1.50	0.10	N8N-CA
8	ND2	8	CA	4.05	0.90	N8ND2-CA
8	ND2	8	CG	1.43	0.10	N8ND2-CG
8	N	9	CA	4.91	2.64	N8N-G9CA
8	N	55	CB	5.28	4.28	N8N-T55CB
8	ND2	55	CB	5.28	2.29	N8ND2-T55CB
8	ND2	55	CG2	3.80	1.10	N8ND2-T55CG2
8	ND2	55	CG2	4.39	3.39	N8ND2-T55CG2
9	N	6	CG2	6.40	5.40	G9N-I6CG2
9	N	7	CA	5.32	4.32	G9N-L7CA
9	N	7	CD2	5.09	4.09	G9N-L7CD2
9	N	8	CA	2.55	0.13	G9N-N8CA
9	N	8	CA	2.46	0.17	G9N-N8CA
9	N	9	CA	1.42	0.10	G9N-CA
9	N	9	CA	1.44	0.10	G9N-CA
9	N	10	CB	6.40	5.40	G9N-K10CB
9	N	12	CD2	5.65	1.47	G9N-L12CD2
9	N	13	CG	4.27	0.10	G9N-K13CG
9	N	13	CE	3.65	0.38	G9N-K13CE
9	N	13	CG	4.92	2.73	G9N-K13CG
9	N	39	CG1	4.85	0.38	G9N-V39CG1
9	N	39	CG1	5.67	0.10	G9N-V39CG1
9	N	54	CG1	5.76	1.03	G9N-V54CG1
9	N	56	CB	4.72	1.75	G9N-E56CB
9	N	56	CD	4.89	1.06	G9N-E56CD
9	N	56	CG	5.07	1.34	G9N-E56CG
10	N	9	CA	2.48	0.10	K10N-G9CA

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
10	N	9	CA	2.58	0.17	K10N-G9CA
10	N	10	CB	2.44	0.10	K10N-CB
10	NZ	10	CD	2.72	1.21	K10NZ-CD
10	NZ	10	CE	1.92	0.92	K10NZ-CE
10	N	10	CG	2.87	0.10	K10N-CG
10	NZ	10	CG	3.89	0.10	K10NZ-CG
10	N	10	CA	1.45	0.10	K10N-CA
10	N	10	CB	2.38	0.10	K10N-CB
10	N	10	CD	4.31	0.10	K10N-CD
10	NZ	10	CD	3.52	1.27	K10NZ-CD
10	N	10	CE	4.66	0.43	K10N-CE
10	NZ	10	CE	1.58	0.10	K10NZ-CE
10	N	10	CG	3.45	1.10	K10N-CG
10	N	13	CE	4.19	0.67	K10N-K13CE
10	NZ	40	CG	5.99	4.99	K10NZ-D40CG
10	NZ	56	CD	5.69	4.69	K10NZ-E56CD
10	N	56	CD	3.60	0.13	K10N-E56CD
10	N	56	CG	3.86	0.16	K10N-E56CG
11	N	10	CA	2.47	0.10	T11N-K10CA
11	N	10	CB	3.31	0.10	T11N-K10CB
11	N	10	CD	5.58	1.45	T11N-K10CD
11	N	10	CG	4.25	0.20	T11N-K10CG
11	N	10	CA	2.53	0.11	T11N-K10CA
11	N	10	CB	3.37	0.10	T11N-K10CB
11	N	10	CD	6.28	1.69	T11N-K10CD
11	N	10	CG	4.72	3.72	T11N-K10CG
11	N	11	CA	1.45	0.10	T11N-CA
11	N	11	CB	2.54	0.10	T11N-CB
11	N	11	CG2	2.80	0.12	T11N-CG2
11	N	11	CA	1.43	0.43	T11N-CA
11	N	11	CB	2.50	0.10	T11N-CB
11	N	11	CG2	3.29	0.28	T11N-CG2
11	N	12	CA	5.07	1.94	T11N-L12CA
11	N	13	CE	4.36	0.67	T11N-K13CE
11	N	39	CG1	6.80	0.38	T11N-V39CG1
11	N	56	CD	5.45	0.99	T11N-E56CD
12	N	9	CA	4.65	2.55	L12N-G9CA
12	N	10	CG	5.88	1.12	L12N-K10CG
12	N	11	CA	2.58	0.13	L12N-T11CA
12	N	11	CB	3.58	2.58	L12N-T11CB
12	N	11	CG2	4.38	0.40	L12N-T11CG2
12	N	11	CA	2.56	0.10	L12N-T11CA
12	N	11	CB	3.58	0.10	L12N-T11CB
12	N	11	CG2	4.94	0.21	L12N-T11CG2
12	N	12	CA	1.43	0.10	L12N-CA
12	N	12	CD2	3.99	0.10	L12N-CD2

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
12	N	12	CB	2.38	0.10	L12N-CB
12	N	12	CD2	4.50	0.17	L12N-CD2
12	N	39	CG1	6.09	0.39	L12N-V39CG1
13	N	7	CD2	4.79	0.16	K13N-L7CD2
13	NZ	7	CD2	6.73	0.16	K13NZ-L7CD2
13	N	9	CA	5.64	4.64	K13N-G9CA
13	N	12	CD2	3.44	0.43	K13N-L12CD2
13	N	12	CG	3.08	1.10	K13N-L12CG
13	N	12	CD2	3.43	1.10	K13N-L12CD2
13	N	13	CA	1.46	0.10	K13N-CA
13	N	13	CB	2.45	0.20	K13N-CB
13	N	13	CD	4.35	1.10	K13N-CD
13	NZ	13	CD	2.66	0.33	K13NZ-CD
13	NZ	13	CE	2.26	1.10	K13NZ-CE
13	N	13	CG	3.06	0.10	K13N-CG
13	NZ	13	CG	4.10	3.10	K13NZ-CG
13	N	13	CA	1.44	0.10	K13N-CA
13	N	13	CB	2.41	0.36	K13N-CB
13	N	13	CD	3.87	0.40	K13N-CD
13	NZ	13	CD	2.91	1.10	K13NZ-CD
13	NZ	13	CE	1.57	0.10	K13NZ-CE
13	N	13	CG	3.22	0.10	K13N-CG
13	NZ	13	CG	3.61	1.10	K13NZ-CG
13	NZ	56	CD	7.18	6.18	K13NZ-E56CD
14	N	6	CD1	6.34	1.15	G14N-I6CD1
14	N	6	CG2	5.46	1.46	G14N-I6CG2
14	N	6	CD1	7.30	1.98	G14N-I6CD1
14	N	7	CA	5.10	4.10	G14N-L7CA
14	N	7	CD2	5.08	1.14	G14N-L7CD2
14	N	7	CB	4.01	1.04	G14N-L7CB
14	N	12	CD2	5.17	0.83	G14N-L12CD2
14	N	13	CA	2.51	0.10	G14N-K13CA
14	N	13	CB	3.37	0.10	G14N-K13CB
14	N	13	CG	3.41	1.10	G14N-K13CG
14	N	13	CA	2.58	0.14	G14N-K13CA
14	N	13	CB	3.21	0.31	G14N-K13CB
14	N	13	CG	4.60	0.10	G14N-K13CG
14	N	14	CA	1.44	0.10	G14N-CA
14	N	14	CA	1.43	0.10	G14N-CA
15	N	6	CD1	5.67	0.16	E15N-I6CD1
15	N	6	CG2	5.57	1.65	E15N-I6CG2
15	N	6	CD1	5.91	1.03	E15N-I6CD1
15	N	7	CD1	3.98	1.10	E15N-L7CD1
15	N	7	CD2	4.76	1.10	E15N-L7CD2
15	N	7	CD1	5.02	1.10	E15N-L7CD1
15	N	14	CA	2.81	0.22	E15N-G14CA

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
15	N	14	CA	2.62	0.14	E15N-G14CA
15	N	15	CA	1.46	0.10	E15N-CA
15	N	15	CB	2.95	0.59	E15N-CB
15	N	15	CG	2.77	0.10	E15N-CG
15	N	15	CA	1.44	0.10	E15N-CA
15	N	15	CB	2.50	0.18	E15N-CB
15	N	15	CD	3.71	0.10	E15N-CD
15	N	15	CG	2.49	1.49	E15N-CG
15	N	16	CG2	6.35	0.96	E15N-T16CG2
16	N	4	CG	4.42	0.28	T16N-K4CG
16	N	5	CD2	5.36	1.10	T16N-L5CD2
16	N	6	CD1	5.74	0.16	T16N-I6CD1
16	N	6	CG2	5.64	1.93	T16N-I6CG2
16	N	6	CD1	5.91	1.03	T16N-I6CD1
16	N	7	CD1	4.06	0.10	T16N-L7CD1
16	N	7	CD1	4.31	0.10	T16N-L7CD1
16	N	15	CA	2.62	0.15	T16N-E15CA
16	N	15	CB	2.81	0.29	T16N-E15CB
16	N	15	CG	3.22	1.11	T16N-E15CG
16	N	15	CA	2.70	0.20	T16N-E15CA
16	N	15	CD	4.24	3.24	T16N-E15CD
16	N	15	CG	3.47	1.10	T16N-E15CG
16	N	16	CG2	2.63	1.37	T16N-CG2
16	N	16	CA	1.38	0.10	T16N-CA
16	N	16	CB	2.43	0.13	T16N-CB
16	N	16	CG2	3.53	0.23	T16N-CG2
17	N	16	CB	3.24	0.10	T17N-T16CB
17	N	16	CG2	3.90	0.10	T17N-T16CG2
17	N	17	CB	2.52	0.17	T17N-CB
17	N	17	CG2	2.56	1.21	T17N-CG2
17	N	17	CB	2.15	0.56	T17N-CB
17	N	17	CG2	3.17	1.10	T17N-CG2
18	N	2	CD	6.62	5.62	T18N-Q2CD
18	N	3	CA	5.03	4.03	T18N-Y3CA
18	N	3	CG	5.56	1.21	T18N-Y3CG
18	N	18	CA	1.43	0.10	T18N-CA
18	N	18	CB	2.47	1.47	T18N-CB
18	N	18	CG2	2.81	0.10	T18N-CG2
18	N	18	CA	1.44	0.10	T18N-CA
18	N	18	CB	2.46	0.10	T18N-CB
18	N	18	CG2	3.30	0.10	T18N-CG2
18	N	19	CD	6.86	0.35	T18N-E19CD
19	N	17	CG2	5.45	0.10	E19N-T17CG2
19	N	18	CA	2.64	0.15	E19N-T18CA
19	N	18	CB	3.30	0.10	E19N-T18CB
19	N	18	CG2	3.07	1.10	E19N-T18CG2

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
19	N	18	CA	2.58	0.15	E19N-T18CA
19	N	18	CB	3.26	0.10	E19N-T18CB
19	N	18	CG2	3.63	0.10	E19N-T18CG2
19	N	19	CA	1.47	0.10	E19N-CA
19	N	19	CA	1.53	0.10	E19N-CA
19	N	19	CD	3.60	1.10	E19N-CD
20	N	20	CB	2.46	0.10	A20N-CB
20	N	20	CA	1.44	0.10	A20N-CA
20	N	20	CB	2.41	0.20	A20N-CB
21	N	1	CE	5.00	0.10	V21N-M1CE
21	N	1	CG	5.88	4.88	V21N-M1CG
21	N	20	CA	2.10	0.13	V21N-A20CA
21	N	20	CB	3.27	0.10	V21N-A20CB
21	N	20	CA	2.70	0.10	V21N-A20CA
21	N	20	CB	3.25	0.10	V21N-A20CB
21	N	21	CG1	2.61	1.19	V21N-CG1
21	N	21	CG2	2.81	1.32	V21N-CG2
21	N	21	CB	2.43	0.10	V21N-CB
21	N	22	CA	3.82	0.89	V21N-D22CA
21	N	25	CG2	4.38	0.10	V21N-T25CG2
22	N	1	CE	5.35	0.84	D22N-M1CE
22	N	20	CA	4.68	2.37	D22N-A20CA
22	N	20	CB	3.92	0.10	D22N-A20CB
22	N	21	CG1	2.93	0.16	D22N-V21CG1
22	N	21	CG2	3.02	0.29	D22N-V21CG2
22	N	22	CA	1.46	0.10	D22N-CA
22	N	22	CB	2.52	0.10	D22N-CB
22	N	22	CA	1.44	0.10	D22N-CA
22	N	22	CB	2.44	0.13	D22N-CB
22	N	25	CG2	4.41	3.41	D22N-T25CG2
23	N	1	CE	4.20	1.04	A23N-M1CE
23	N	22	CA	2.60	0.18	A23N-D22CA
23	N	22	CB	2.93	0.10	A23N-D22CB
23	N	22	CA	2.50	0.16	A23N-D22CA
23	N	22	CB	3.21	0.10	A23N-D22CB
23	N	23	CB	2.49	0.15	A23N-CB
23	N	23	CA	1.44	0.10	A23N-CA
23	N	23	CB	2.34	0.10	A23N-CB
23	N	26	CB	6.01	2.10	A23N-A26CB
24	N	24	CA	1.51	0.10	A24N-CA
24	N	24	CB	2.75	0.23	A24N-CB
24	N	24	CA	1.53	0.10	A24N-CA
24	N	24	CB	2.35	0.10	A24N-CB
24	N	25	CA	4.68	1.60	A24N-T25CA
25	N	24	CA	2.90	0.20	T25N-A24CA
25	N	24	CB	3.82	1.10	T25N-A24CB

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
25	N	24	CA	2.80	0.10	T25N-A24CA
25	N	24	CB	3.39	0.10	T25N-A24CB
25	N	25	CA	1.44	0.10	T25N-CA
25	N	25	CB	2.50	0.20	T25N-CB
25	N	25	CG2	2.72	1.10	T25N-CG2
25	N	25	CA	1.49	0.10	T25N-CA
25	N	25	CB	2.44	0.15	T25N-CB
25	N	25	CG2	3.51	0.10	T25N-CG2
25	N	26	CA	4.24	1.13	T25N-A26CA
26	N	20	CB	4.43	0.10	A26N-A20CB
26	N	20	CB	4.08	0.45	A26N-A20CB
26	N	25	CA	2.73	0.21	A26N-T25CA
26	N	25	CB	3.15	0.37	A26N-T25CB
26	N	25	CA	2.53	0.15	A26N-T25CA
26	N	25	CB	3.48	0.43	A26N-T25CB
26	N	26	CB	2.46	0.10	A26N-CB
26	N	26	CA	1.45	0.10	A26N-CA
26	N	26	CB	2.42	0.13	A26N-CB
26	N	27	CG	5.36	0.10	A26N-E27CG
26	N	27	CD	6.21	0.10	A26N-E27CD
27	N	26	CB	3.34	0.10	E27N-A26CB
27	N	26	CA	2.51	0.16	E27N-A26CA
27	N	26	CB	3.36	0.31	E27N-A26CB
27	N	27	CA	1.48	0.10	E27N-CA
27	N	27	CB	2.42	0.15	E27N-CB
27	N	27	CG	3.30	0.10	E27N-CG
27	N	27	CA	1.44	0.10	E27N-CA
27	N	27	CB	2.42	0.11	E27N-CB
27	N	27	CD	4.94	0.10	E27N-CD
27	N	28	CD	5.96	1.11	E27N-K28CD
27	N	28	CE	6.61	5.61	E27N-K28CE
27	N	29	CG2	5.39	2.05	E27N-V29CG2
27	N	30	CG	4.82	0.34	E27N-F30CG
28	NZ	24	CB	6.94	5.94	K28NZ-A24CB
28	NZ	25	CG2	6.07	0.10	K28NZ-T25CG2
28	N	26	CB	5.74	4.74	K28N-A26CB
28	N	26	CB	5.28	0.98	K28N-A26CB
28	N	27	CA	2.53	0.13	K28N-E27CA
28	N	27	CB	2.99	0.26	K28N-E27CB
28	N	27	CG	3.28	0.11	K28N-E27CG
28	N	27	CA	2.49	0.10	K28N-E27CA
28	N	27	CB	3.20	0.10	K28N-E27CB
28	N	27	CD	4.25	0.10	K28N-E27CD
28	N	28	CA	1.47	0.10	K28N-CA
28	N	28	CB	2.43	0.10	K28N-CB
28	N	28	CD	4.32	0.29	K28N-CD

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
28	NZ	28	CD	2.88	0.10	K28NZ-CD
28	N	28	CE	5.45	1.95	K28N-CE
28	NZ	28	CE	1.88	0.10	K28NZ-CE
28	N	28	CG	2.67	0.22	K28N-CG
28	N	28	CA	1.44	0.10	K28N-CA
28	N	28	CB	2.41	0.10	K28N-CB
28	N	28	CD	4.58	0.10	K28N-CD
28	NZ	28	CD	3.29	1.10	K28NZ-CD
28	N	28	CE	5.95	2.09	K28N-CE
28	NZ	28	CE	1.87	0.10	K28NZ-CE
28	N	28	CG	3.14	0.28	K28N-CG
28	NZ	28	CG	4.19	0.28	K28NZ-CG
28	N	29	CG1	4.67	1.74	K28N-V29CG1
28	N	29	CG2	5.28	1.86	K28N-V29CG2
29	N	28	CA	2.29	0.10	V29N-K28CA
29	N	28	CB	3.17	0.12	V29N-K28CB
29	N	28	CD	6.84	2.84	V29N-K28CD
29	N	28	CA	2.39	0.10	V29N-K28CA
29	N	28	CB	3.15	0.14	V29N-K28CB
29	N	28	CG	4.41	0.30	V29N-K28CG
29	N	29	CA	1.49	0.10	V29N-CA
29	N	29	CG1	2.96	1.10	V29N-CG1
29	N	29	CG2	2.69	0.10	V29N-CG2
29	N	29	CG2	2.75	0.50	V29N-CG2
30	N	29	CG1	2.81	1.10	F30N-V29CG1
30	N	29	CG2	4.29	0.26	F30N-V29CG2
30	N	29	CG1	3.57	0.24	F30N-V29CG1
30	N	30	CB	2.47	0.10	F30N-CB
30	N	30	CA	1.45	0.10	F30N-CA
30	N	30	CG	2.99	0.10	F30N-CG
30	N	33	CB	3.82	0.28	F30N-Y33CB
31	NZ	27	CG	3.67	1.10	K31NZ-E27CG
31	N	27	CG	4.19	1.10	K31N-E27CG
31	NZ	27	CD	4.00	0.10	K31NZ-E27CD
31	N	30	CB	3.06	0.10	K31N-F30CB
31	N	30	CA	2.56	0.10	K31N-F30CA
31	N	30	CG	4.42	0.10	K31N-F30CG
31	N	31	CA	1.47	0.10	K31N-CA
31	N	31	CB	2.62	0.10	K31N-CB
31	NZ	31	CD	2.52	0.15	K31NZ-CD
31	NZ	31	CE	1.61	0.10	K31NZ-CE
31	N	31	CG	2.43	1.16	K31N-CG
31	N	31	CA	1.45	0.10	K31N-CA
31	N	31	CB	2.35	0.10	K31N-CB
31	NZ	31	CD	2.32	0.10	K31NZ-CD
31	NZ	31	CE	1.90	0.90	K31NZ-CE

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
31	N	31	CG	2.92	1.92	K31N-CG
31	NZ	31	CG	3.76	0.10	K31NZ-CG
31	NZ	43	CD2	5.28	1.38	K31NZ-W43CD2
31	N	43	CZ2	4.49	0.25	K31N-W43CZ2
31	N	43	CZ3	4.53	0.10	K31N-W43CZ3
31	NZ	43	CZ3	6.38	0.10	K31NZ-W43CZ3
32	N	31	CB	3.12	0.10	Q32N-K31CB
32	N	31	CA	2.53	0.12	Q32N-K31CA
32	N	32	CA	1.42	0.10	Q32N-CA
32	NE2	32	CB	2.43	1.10	Q32NE2-CB
32	NE2	32	CD	1.70	0.10	Q32NE2-CD
32	NE2	32	CG	2.59	0.12	Q32NE2-CG
32	N	32	CA	1.47	0.10	Q32N-CA
32	N	32	CB	2.24	0.12	Q32N-CB
32	NE2	32	CB	3.91	0.37	Q32NE2-CB
32	N	54	CG1	6.30	5.30	Q32N-V54CG1
33	N	33	CB	2.47	0.34	Y33N-CB
33	N	33	CA	1.44	0.10	Y33N-CA
33	N	33	CG	3.47	0.10	Y33N-CG
34	N	30	CG	5.86	1.46	A34N-F30CG
34	N	33	CB	3.44	0.64	A34N-Y33CB
34	N	33	CA	2.39	0.15	A34N-Y33CA
34	N	33	CG	3.35	0.10	A34N-Y33CG
34	N	34	CA	1.51	0.10	A34N-CA
34	N	34	CB	2.44	0.10	A34N-CB
34	N	34	CA	1.46	0.10	A34N-CA
34	N	34	CB	2.42	0.10	A34N-CB
34	N	35	CA	3.57	0.58	A34N-N35CA
34	N	54	CG1	6.17	5.17	A34N-V54CG1
35	N	34	CA	2.81	0.10	N35N-A34CA
35	N	34	CB	3.29	0.10	N35N-A34CB
35	N	34	CA	2.50	0.12	N35N-A34CA
35	N	34	CB	3.32	0.10	N35N-A34CB
35	N	35	CA	1.47	0.10	N35N-CA
35	N	35	CB	2.47	0.16	N35N-CB
35	ND2	35	CB	3.54	1.27	N35ND2-CB
35	N	35	CG	3.53	0.10	N35N-CG
35	ND2	35	CG	1.87	0.87	N35ND2-CG
35	N	35	CA	1.41	0.10	N35N-CA
35	N	35	CB	2.42	0.10	N35N-CB
35	ND2	35	CB	3.74	1.10	N35ND2-CB
35	ND2	35	CG	1.88	0.88	N35ND2-CG
36	N	35	CA	2.59	0.15	D36N-N35CA
36	N	35	CB	3.02	0.10	D36N-N35CB
36	N	35	CA	2.60	0.10	D36N-N35CA
36	N	35	CB	3.15	0.13	D36N-N35CB

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
36	N	36	CA	1.45	0.10	D36N-CA
36	N	36	CB	2.41	0.10	D36N-CB
36	N	36	CA	1.44	0.10	D36N-CA
36	N	36	CB	2.44	0.10	D36N-CB
36	N	36	CG	2.56	0.10	D36N-CG
36	N	37	CG	5.05	2.33	D36N-N37CG
37	ND2	12	CD1	3.06	0.10	N37ND2-L12CD1
37	ND2	12	CD2	5.68	1.54	N37ND2-L12CD2
37	N	33	CG	5.27	0.11	N37N-Y33CG
37	ND2	33	CG	3.86	1.10	N37ND2-Y33CG
37	N	36	CA	2.94	1.18	N37N-D36CA
37	N	36	CB	3.38	0.30	N37N-D36CB
37	ND2	36	CB	5.05	1.82	N37ND2-D36CB
37	N	36	CA	2.51	0.18	N37N-D36CA
37	N	36	CB	3.46	0.10	N37N-D36CB
37	N	37	CA	1.48	0.10	N37N-CA
37	N	37	CB	2.39	0.25	N37N-CB
37	ND2	37	CB	2.63	1.63	N37ND2-CB
37	ND2	37	CG	1.42	0.10	N37ND2-CG
37	N	37	CA	1.48	0.10	N37N-CA
37	ND2	37	CA	4.29	1.20	N37ND2-CA
37	N	37	CB	2.27	0.10	N37N-CB
37	ND2	37	CB	2.58	0.11	N37ND2-CB
37	N	37	CG	2.40	1.21	N37N-CG
37	ND2	37	CG	1.51	0.10	N37ND2-CG
37	N	38	CA	4.36	1.53	N37N-G38CA
37	N	39	CG1	5.64	0.39	N37N-V39CG1
38	N	12	CD1	4.31	0.10	G38N-L12CD1
38	N	37	CA	2.74	0.18	G38N-N37CA
38	N	37	CB	3.70	2.70	G38N-N37CB
38	N	37	CA	2.59	0.21	G38N-N37CA
38	N	37	CB	3.88	1.10	G38N-N37CB
38	N	38	CA	1.49	0.10	G38N-CA
38	N	38	CA	1.43	0.10	G38N-CA
39	N	34	CB	4.46	0.86	V39N-A34CB
39	N	37	CG	6.32	4.88	V39N-N37CG
39	N	38	CA	2.53	0.12	V39N-G38CA
39	N	38	CA	2.60	0.10	V39N-G38CA
39	N	39	CA	1.43	0.10	V39N-CA
39	N	39	CG1	2.81	0.10	V39N-CG1
39	N	39	CG1	3.11	0.34	V39N-CG1
39	N	40	CG	6.60	0.16	V39N-D40CG
39	N	56	CD	4.83	0.74	V39N-E56CD
40	N	10	CE	5.48	1.21	D40N-K10CE
40	N	39	CA	2.35	0.11	D40N-V39CA
40	N	39	CG1	3.26	2.26	D40N-V39CG1

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
40	N	39	CG1	3.81	1.10	D40N-V39CG1
40	N	40	CA	1.50	0.10	D40N-CA
40	N	40	CB	2.51	0.10	D40N-CB
40	N	40	CG	2.82	1.10	D40N-CG
40	N	40	CA	1.48	0.10	D40N-CA
40	N	40	CB	2.46	0.18	D40N-CB
40	N	40	CG	4.51	1.32	D40N-CG
40	N	41	CA	4.34	1.10	D40N-G41CA
40	N	56	CD	3.42	0.20	D40N-E56CD
41	N	34	CB	5.30	1.79	G41N-A34CB
41	N	40	CA	2.62	0.10	G41N-D40CA
41	N	40	CB	3.60	0.17	G41N-D40CB
41	N	40	CG	3.57	0.10	G41N-D40CG
41	N	40	CA	2.59	0.10	G41N-D40CA
41	N	40	CB	3.64	0.46	G41N-D40CB
41	N	40	CG	4.23	0.15	G41N-D40CG
41	N	41	CA	1.46	0.10	G41N-CA
41	N	41	CA	1.47	0.10	G41N-CA
41	N	54	CG1	6.13	2.85	G41N-V54CG1
41	N	54	CG2	3.05	0.10	G41N-V54CG2
41	N	54	CG2	2.93	0.10	G41N-V54CG2
41	N	56	CB	4.24	0.20	G41N-E56CB
41	N	56	CD	4.50	0.30	G41N-E56CD
41	N	56	CG	5.41	1.40	G41N-E56CG
42	N	41	CA	2.68	0.14	E42N-G41CA
42	N	41	CA	2.63	0.10	E42N-G41CA
42	N	42	CA	1.42	0.10	E42N-CA
42	N	42	CG	2.56	0.12	E42N-CG
42	N	42	CA	1.06	0.06	E42N-CA
42	N	42	CB	2.51	0.14	E42N-CB
43	NE1	31	CG	4.40	0.10	W43NE1-K31CG
43	NE1	34	CB	5.90	3.20	W43NE1-A34CB
43	N	42	CA	2.61	0.20	W43N-E42CA
43	N	42	CB	3.41	0.29	W43N-E42CB
43	N	43	CA	1.43	0.10	W43N-CA
43	N	43	CD1	3.70	0.39	W43N-CD1
43	NE1	43	CD1	1.46	0.10	W43NE1-CD1
43	N	43	CD2	5.02	3.05	W43N-CD2
43	NE1	43	CD2	2.26	0.10	W43NE1-CD2
43	NE1	43	CZ2	2.52	0.17	W43NE1-CZ2
43	NE1	43	CZ3	4.10	0.10	W43NE1-CZ3
43	N	43	CZ3	6.02	0.10	W43N-CZ3
43	N	44	CG2	5.42	4.42	W43N-T44CG2
43	NE1	54	CG1	5.00	0.85	W43NE1-V54CG1
43	NE1	54	CG2	3.21	0.10	W43NE1-V54CG2
43	N	54	CG2	4.94	0.10	W43N-V54CG2

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
43	N	55	CG2	5.72	0.10	W43N-T55CG2
44	N	43	CB	2.81	0.10	T44N-W43CB
44	N	43	CZ3	6.04	0.10	T44N-W43CZ3
44	N	44	CA	1.45	0.10	T44N-CA
44	N	44	CB	2.47	0.38	T44N-CB
44	N	44	CG2	2.71	0.11	T44N-CG2
44	N	44	CA	1.43	0.10	T44N-CA
44	N	44	CB	2.45	0.10	T44N-CB
44	N	44	CG2	3.01	0.96	T44N-CG2
45	N	44	CA	2.58	1.58	Y45N-T44CA
45	N	44	CB	3.22	0.10	Y45N-T44CB
45	N	44	CA	2.59	0.10	Y45N-T44CA
45	N	44	CB	3.31	0.10	Y45N-T44CB
45	N	45	CB	2.35	0.10	Y45N-CB
45	N	45	CA	1.44	0.10	Y45N-CA
45	N	45	CG	3.67	0.29	Y45N-CG
45	N	52	CG	5.72	1.15	Y45N-F52CG
46	N	45	CA	2.56	0.14	D46N-Y45CA
46	N	45	CG	3.27	0.10	D46N-Y45CG
46	N	46	CA	1.44	0.10	D46N-CA
46	N	46	CB	2.46	0.10	D46N-CB
46	N	46	CA	1.45	0.10	D46N-CA
46	N	46	CB	2.48	0.22	D46N-CB
46	N	46	CG	3.53	0.19	D46N-CG
46	N	51	CB	4.89	1.00	D46N-T51CB
46	N	51	CB	5.28	3.00	D46N-T51CB
46	N	52	CG	5.25	1.11	D46N-F52CG
47	N	45	CA	5.95	4.95	D47N-Y45CA
47	N	45	CG	4.19	0.10	D47N-Y45CG
47	N	46	CA	2.76	0.19	D47N-D46CA
47	N	46	CA	2.61	0.10	D47N-D46CA
47	N	46	CB	3.90	0.10	D47N-D46CB
47	N	46	CG	3.24	0.10	D47N-D46CG
47	N	47	CA	1.51	0.10	D47N-CA
47	N	47	CB	2.46	0.38	D47N-CB
47	N	47	CA	1.41	0.10	D47N-CA
47	N	47	CB	3.00	1.17	D47N-CB
47	N	47	CG	3.76	0.51	D47N-CG
47	N	48	CB	5.36	1.05	D47N-A48CB
47	N	48	CA	4.22	1.45	D47N-A48CA
48	N	46	CA	4.20	0.98	A48N-D46CA
48	N	46	CG	3.42	0.10	A48N-D46CG
48	N	47	CA	3.48	1.65	A48N-D47CA
48	N	47	CB	3.70	0.50	A48N-D47CB
48	N	47	CA	2.82	0.41	A48N-D47CA
48	N	47	CB	4.32	1.18	A48N-D47CB

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
48	N	48	CA	1.50	0.10	A48N-CA
48	N	48	CB	2.50	0.10	A48N-CB
48	N	48	CA	1.46	0.10	A48N-CA
48	N	48	CB	2.45	0.10	A48N-CB
48	N	49	CG2	5.29	0.38	A48N-T49CG2
49	N	46	CG	3.67	0.10	T49N-D46CG
49	N	47	CA	5.95	4.95	T49N-D47CA
49	N	48	CA	2.81	0.18	T49N-A48CA
49	N	48	CB	3.39	0.20	T49N-A48CB
49	N	48	CA	2.49	0.10	T49N-A48CA
49	N	48	CB	3.38	0.10	T49N-A48CB
49	N	49	CB	2.50	0.28	T49N-CB
49	N	49	CG2	2.88	0.25	T49N-CG2
49	N	49	CA	1.44	0.10	T49N-CA
49	N	49	CB	2.45	0.10	T49N-CB
49	N	49	CG2	3.38	0.10	T49N-CG2
49	N	50	CB	5.28	1.57	T49N-K50CB
49	N	50	CD	6.06	5.06	T49N-K50CD
49	N	50	CA	4.95	1.30	T49N-K50CA
49	N	50	CG	4.88	0.90	T49N-K50CG
49	N	51	CB	5.95	1.79	T49N-T51CB
50	NZ	1	CE	3.83	0.10	K50NZ-M1CE
50	NZ	3	CG	6.69	5.69	K50NZ-Y3CG
50	NZ	23	CB	6.58	2.81	K50NZ-A23CB
50	NZ	48	CB	6.83	0.86	K50NZ-A48CB
50	N	49	CB	3.81	0.35	K50N-T49CB
50	N	49	CG2	5.16	0.88	K50N-T49CG2
50	N	49	CB	3.84	0.10	K50N-T49CB
50	N	49	CG2	5.55	0.64	K50N-T49CG2
50	N	50	CA	1.42	0.10	K50N-CA
50	N	50	CB	2.51	0.23	K50N-CB
50	NZ	50	CB	4.50	0.80	K50NZ-CB
50	N	50	CD	3.32	0.10	K50N-CD
50	NZ	50	CD	2.26	0.13	K50NZ-CD
50	NZ	50	CE	1.59	0.10	K50NZ-CE
50	N	50	CG	2.70	0.29	K50N-CG
50	NZ	50	CG	3.74	0.27	K50NZ-CG
50	N	50	CA	1.44	0.10	K50N-CA
50	N	50	CB	2.43	0.10	K50N-CB
50	NZ	50	CB	4.66	0.53	K50NZ-CB
50	N	50	CD	3.40	0.10	K50N-CD
50	NZ	50	CD	2.63	0.10	K50NZ-CD
50	NZ	50	CE	2.20	1.10	K50NZ-CE
50	N	50	CG	2.91	0.58	K50N-CG
50	N	51	CB	5.16	1.74	K50N-T51CB
50	N	51	CA	4.63	3.27	K50N-T51CA

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
50	N	51	CB	5.51	0.79	K50N-T51CB
51	N	3	CG	6.08	2.37	T51N-Y3CG
51	N	4	CG	5.30	2.33	T51N-K4CG
51	N	45	CG	5.08	0.55	T51N-Y45CG
51	N	49	CB	5.23	1.16	T51N-T49CB
51	N	49	CG2	5.12	0.90	T51N-T49CG2
51	N	49	CB	4.81	0.56	T51N-T49CB
51	N	49	CG2	7.41	6.41	T51N-T49CG2
51	N	50	CB	4.24	0.68	T51N-K50CB
51	N	50	CB	4.15	1.07	T51N-K50CB
51	N	50	CG	4.96	0.35	T51N-K50CG
51	N	51	CA	1.45	0.10	T51N-CA
51	N	51	CB	2.50	0.11	T51N-CB
51	N	51	CG2	3.23	1.10	T51N-CG2
51	N	51	CA	1.43	0.10	T51N-CA
51	N	51	CB	2.47	0.10	T51N-CB
51	N	51	CG2	4.02	0.12	T51N-CG2
52	N	5	CD2	4.87	0.10	F52N-L5CD2
52	N	6	CD1	5.43	1.14	F52N-I6CD1
52	N	6	CG2	5.56	2.28	F52N-I6CG2
52	N	6	CD1	5.65	0.64	F52N-I6CD1
52	N	45	CG	4.93	0.52	F52N-Y45CG
52	N	51	CA	2.71	0.16	F52N-T51CA
52	N	51	CB	3.68	0.10	F52N-T51CB
52	N	51	CG2	3.18	0.15	F52N-T51CG2
52	N	51	CA	2.59	0.15	F52N-T51CA
52	N	51	CB	3.63	0.27	F52N-T51CB
52	N	51	CG2	3.37	0.10	F52N-T51CG2
52	N	52	CB	2.32	0.10	F52N-CB
52	N	52	CA	1.43	0.10	F52N-CA
52	N	52	CG	2.71	0.14	F52N-CG
53	N	5	CD2	3.92	2.92	T53N-L5CD2
53	N	5	CD2	3.70	0.10	T53N-L5CD2
53	N	6	CG1	5.40	1.12	T53N-I6CG1
53	N	6	CG2	5.81	4.81	T53N-I6CG2
53	N	6	CD1	5.35	3.54	T53N-I6CD1
53	N	43	CZ3	4.90	3.90	T53N-W43CZ3
53	N	44	CB	4.79	0.59	T53N-T44CB
53	N	44	CG2	3.66	0.10	T53N-T44CG2
53	N	52	CA	2.64	0.16	T53N-F52CA
53	N	53	CA	1.49	0.10	T53N-CA
53	N	53	CG2	2.97	0.10	T53N-CG2
53	N	53	CA	1.43	0.10	T53N-CA
53	N	53	CG2	3.12	0.12	T53N-CG2
53	N	54	CG1	6.13	2.44	T53N-V54CG1
54	N	5	CD2	3.77	0.10	V54N-L5CD2

Residue i	Atom	Residue j	Atom	Distance (Å)	Uncertainty (Å)	Label
54	N	5	CD2	3.67	0.10	V54N-L5CD2
54	N	6	CD1	6.79	1.17	V54N-I6CD1
54	N	6	CB	5.72	0.10	V54N-I6CB
54	N	6	CD1	6.82	1.69	V54N-I6CD1
54	N	7	CA	3.85	1.86	V54N-L7CA
54	N	43	CZ3	4.55	0.10	V54N-W43CZ3
54	N	53	CA	2.82	0.10	V54N-T53CA
54	N	54	CA	1.45	0.10	V54N-CA
54	N	54	CG1	3.04	0.12	V54N-CG1
54	N	54	CG2	3.09	1.10	V54N-CG2
54	N	54	CG1	3.18	2.18	V54N-CG1
55	N	54	CA	2.66	0.15	T55N-V54CA
55	N	54	CG1	4.15	0.10	T55N-V54CG1
55	N	54	CG2	2.92	1.92	T55N-V54CG2
55	N	54	CG1	4.20	0.10	T55N-V54CG1
55	N	55	CA	1.43	0.10	T55N-CA
55	N	55	CB	2.50	0.10	T55N-CB
55	N	55	CG2	2.90	0.24	T55N-CG2
55	N	55	CA	1.46	0.10	T55N-CA
55	N	55	CB	2.48	0.15	T55N-CB
55	N	55	CG2	3.46	0.10	T55N-CG2
55	N	56	CD	6.50	2.64	T55N-E56CD
55	N	56	CG	6.02	4.84	T55N-E56CG
56	N	10	CD	5.71	1.51	E56N-K10CD
56	N	10	CG	6.40	0.12	E56N-K10CG
56	N	54	CG1	6.13	2.85	E56N-V54CG1
56	N	55	CA	2.66	0.16	E56N-T55CA
56	N	55	CB	3.67	0.10	E56N-T55CB
56	N	55	CG2	2.89	1.52	E56N-T55CG2
56	N	55	CA	2.61	0.18	E56N-T55CA
56	N	55	CB	3.66	0.10	E56N-T55CB
56	N	55	CG2	3.47	1.10	E56N-T55CG2
56	N	56	CA	1.44	0.10	E56N-CA
56	N	56	CB	2.96	1.10	E56N-CB
56	N	56	CG	2.50	0.10	E56N-CG
56	N	56	CA	1.44	0.28	E56N-CA
56	N	56	CB	2.45	0.10	E56N-CB
56	N	56	CG	2.48	0.25	E56N-CG

Table S3. Dihedral Restraints

Residue	Angle	Value	Error
2	Φ	-109	17
2	Ψ	136	13
3	Φ	-130	14
3	Ψ	153	15
4	Φ	-137	17
4	Ψ	136	7
5	Φ	-115	16
5	Ψ	122	16
6	Φ	-108	6
6	Ψ	120	12
7	Φ	-103	9
7	Ψ	119	11
8	Φ	-100	17
8	Ψ	142	26
11	Φ	-94	17
11	Ψ	-6	14
12	Φ	-113	25
12	Ψ	124	27
13	Φ	-134	10
13	Ψ	156	16
14	Φ	-153	15
14	Ψ	159	23
15	Φ	-129	12
15	Ψ	151	12
16	Φ	-125	21
16	Ψ	153	23
17	Φ	-134	10
17	Ψ	152	20
18	Φ	-130	25
18	Ψ	137	14
19	Φ	-117	10
19	Ψ	122	16
20	Φ	-124	28
20	Ψ	160	16
23	Φ	-63	10
23	Ψ	-35	11
24	Φ	-65	6
24	Ψ	-38	7
25	Φ	-66	9
25	Ψ	-38	8
26	Φ	-62	5
26	Ψ	-41	3
27	Φ	-66	8
27	Ψ	-37	17

Residue	Angle	Value	Error
28	Φ	-65	4
28	Ψ	-41	5
29	Φ	-64	4
29	Ψ	-46	4
30	Φ	-67	4
30	Ψ	-35	7
31	Φ	-66	7
31	Ψ	-41	10
32	Φ	-66	7
32	Ψ	-43	9
33	Φ	-67	5
33	Ψ	-37	9
34	Φ	-66	5
34	Ψ	-42	4
35	Φ	-64	7
35	Ψ	-37	11
36	Φ	-61	5
36	Ψ	-31	8
37	Φ	-102	16
37	Ψ	8	16
38	Φ	83	11
38	Ψ	14	9
39	Φ	-101	20
39	Ψ	125	15
40	Φ	-98	27
40	Ψ	139	28
42	Φ	-98	22
42	Ψ	133	16
43	Φ	-122	16
43	Ψ	160	10
44	Φ	-133	23
44	Ψ	152	17
45	Φ	-119	28
45	Ψ	126	24
46	Φ	-105	18
46	Ψ	140	26
48	Φ	-66	13
48	Ψ	-21	15
49	Φ	-110	9
49	Ψ	10	13
51	Φ	-105	43
51	Ψ	134	16
52	Φ	-121	13
52	Ψ	150	16
53	Φ	-133	11
53	Ψ	144	17

Residue	Angle	Value	Error
54	Φ	-131	16
54	Ψ	139	14
55	Φ	-110	14
55	Ψ	128	12

Table S4. XPLOR-NIH Calculation Energies

Orthorhombic Refine	Average (kcal/mol)	Standard Deviation (kcal/mol)
ANGL	385	20
BOND	225	6
CDIH	35	5
IMPR	50	9
Distance	1391	16
posDiff	236	42
VDW	148	12
TOTAL	2470	24
Trigonal Refine		
ANGL	623	13
BOND	169	6
CDIH	61	5
IMPR	93	7
Distance	1215	27
posDiff	150	23
VDW	500	19
TOTAL	2811	27
***De novo* Annealing**		
ANGL	909	23
BOND	421	7
CDIH	107	5
IM Distance	198	12
IMPR	156	5
Distance	1730	17
posDiff	190	7
VDW	773	24
TOTAL	4484	20

References:

(1) Franks, W. T.; Wylie, B. J.; Schmidt, H. L. F.; Nieuwkoop, A. J.; Mayrhofer, R. M.; Shah, G. J.; Graesser, D. T.; Rienstra, C. M. *Proc. Nat. Acad. Sci. U.S.A.* **2008**, *105*, 4621.

(2) Nieuwkoop, A. J.; Wylie, B. J.; Franks, W. T.; Shah, G. J.; Rienstra, C. M. *J. Chem. Phys.* **2009**, *131*, 095101.

(3) Franks, W. T.; Wylie, B. J.; Stellfox, S. A.; Rienstra, C. M. *J. Am. Chem. Soc.* **2006**, *128*, 3154.

(4) Frericks Schmidt, H. L.; Sperling, L. J.; Gao, Y. G.; Wylie, B. J.; Boettcher, J. M.; Wilson, S. R.; Rienstra, C. M. *J. Phys. Chem. B* **2007**, *111*, 14362.

(5) Guex, N.: Peitsch, M.C. *Electrophoresis* **1997**, *18*, 2714.

(6) Schwieters, C. D.; Clore, G. M., *J. Magn. Reson.* **2001,** *149*, 239.

(7) Schwieters, C. D.; Kuszewski, J. J.; Tjandra, N.; Clore, G. M. *J. Magn. Reson.* **2003**, *160*, 65.