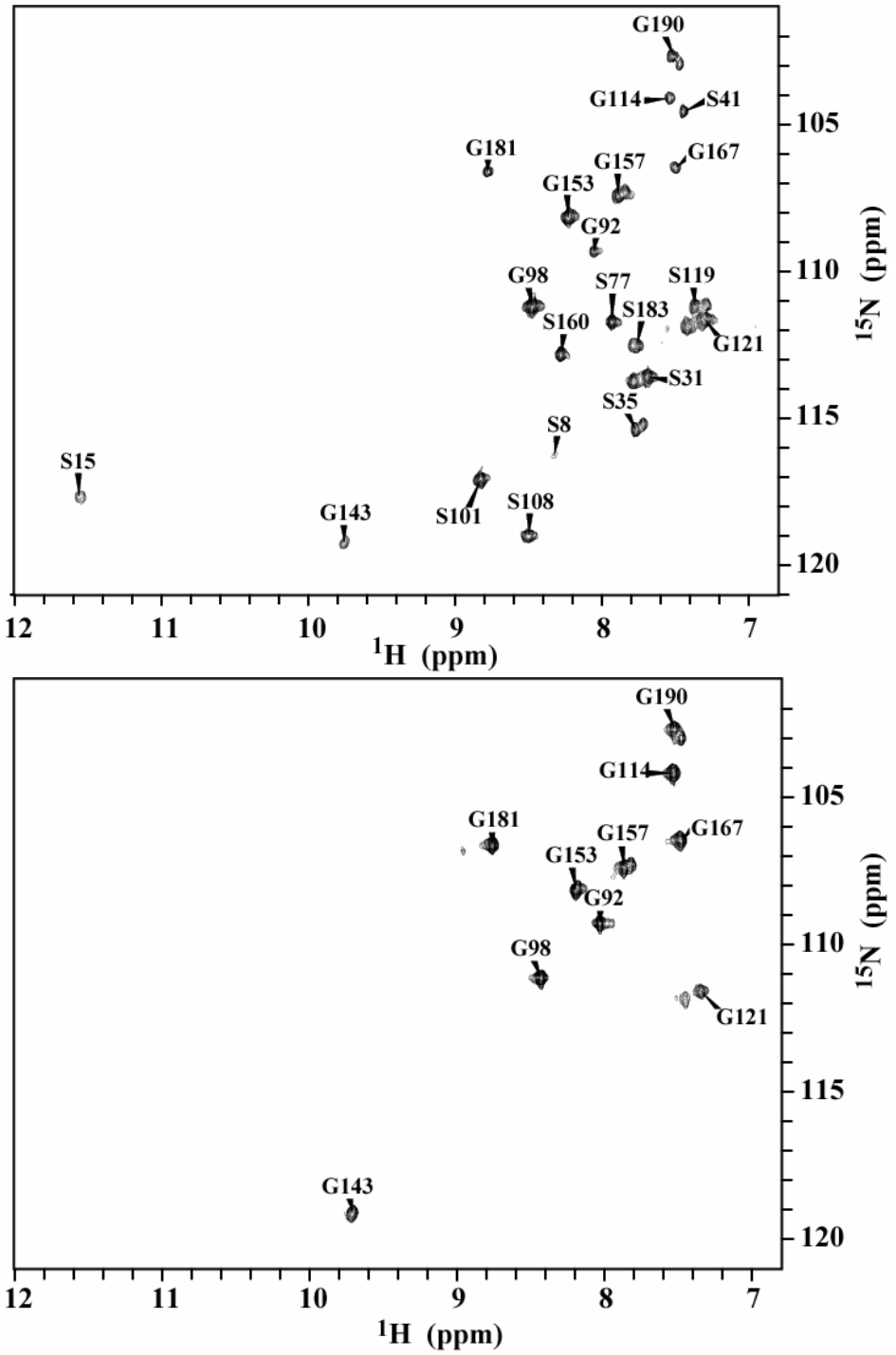

Figure S1. $^{1}H\{^{15}N\}$ HSQC of *pa*-HO-N_3 labeled with ^{15}N-Gly and ^{15}N-Ser (Top) and labeled only with ^{15}N-Gly (Bottom). The protein used to obtain the spectrum shown on the top panel was produced in an analogous manner to other selectively labeled protein samples in M9 medium containing [U-^{15}N]-Gly. Labeling patterns giving rise to the spectrum shown on the top panel resulted when low amounts of L-Ser where present in the expression media, see Experimental Methods. Increasing the concentration of L-Ser in the medium while maintaining that of [U-^{15}N]-Gly constant, alleviated isotopic scrambling, as evidenced from the lack of cross-peaks originating from Ser residues in the spectrum shown on the bottom panel.

Strategy for Sequential Resonance Assignments. Assignment of resonances not strongly affected by the iron paramagnetism was carried out with the aid of heteronuclear correlation experiments following established procedures (see for example ref 54). The process started with the analysis of a CBCA(CO)NH spectrum by which correlations between NH resonances of a given residue and the $^{13}C^{\beta}$ and/or $^{13}C^{\alpha}$ resonances of the preceding residue were obtained. Our approach took advantage of the fact that correlations to C^{β} and/or C^{α} of Ala, Gly, Ser or Thr residues were identified with relative ease due to their characteristic patterns of $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ chemical shifts. For instance, Ala exhibits characteristic $^{13}C^{\beta}$ shifts near 15 ppm. Thus, a $^{13}C^{\beta}$ cross peak at ~15 ppm accompanied by a $^{13}C^{\alpha}$ cross peak near 53 ppm in the CBCA(CO)NH spectrum is diagnostic of Ala. Similarly, a $^{13}C^{\alpha}$ cross-peak near 45 ppm not accompanied by a $^{13}C^{\beta}$ cross-peak is suggestive of Gly. Following these tentative identifications, amino acid pairs comprising any combination of Ala, Gly, Ser or Thr spin systems were identified. Specifically, the pair Gly-Ala was initially identified from analysis of HNCA, HN(CO)CA, HNCACB and CBCA(CO)NH spectra. HNCA and HNCACB spectra provide intra- and inter-residue correlations between NH nuclei and $^{13}C^{\beta}$ and/or $^{13}C^{\alpha}$ nuclei of the same and preceding residue, respectively, whereas HN(CO)CA and CBCA(CO)NH spectra show exclusively inter-residue correlations between the amide NH with the $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ of the preceding residue. The pair Gly-Ala occurs in three distinct places in the sequence of *pa*-HO and involves fragments G125-A126, G143-A144 and G181-A182. Analysis of the above-mentioned spectra in search of patterns suggesting the presence of Gly-Ala amino acid pairs returned two such correlations. With this information at hand, the analysis was extended to include residues following Ala. Inspection of the amino acid sequence revealed two sequences, G125-A126-A127 and G181-A182-S183, which are expected to show characteristic chemical shift patterns, and the sequence G143-A144-R145. Analysis of the aforementioned 3D spectra allowed unambiguous assignment of the fragment G181-A182-S183 on the basis of inter-residue correlations between S183 NH and the $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ peaks of A182 and intra-residue correlations between the same NH nuclei and a set of $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ peaks characteristic of Ser residues (Figure S2). The G143-A144-R145 sequence

was unambiguously assigned from inter-residue correlations between R145 NH and the $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ peaks of A144 and from inter-residue correlations between the same N-H and the atypical set of $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ peaks. This approach was used to assign other regions of the protein sequence and yielded more than 80 % of the backbone assignments. Subsequently, these assignments were confirmed and extended by analyzing the HNCO and (HCA)CO(CA)NH spectra. These spectra provide sequential intra- and inter-residue [(HCA)CO(CA)NH] or exclusively inter-residue (HNCO) correlations between NH and ^{13}CO nuclei. Strip plots showing a fragment of the protein sequence assigned in this fashion are shown in Figure S3. The information obtained from these set of 3D triple-resonance spectra was complemented with data obtained from a ^{15}N-separated NOESY-HSQC spectrum.

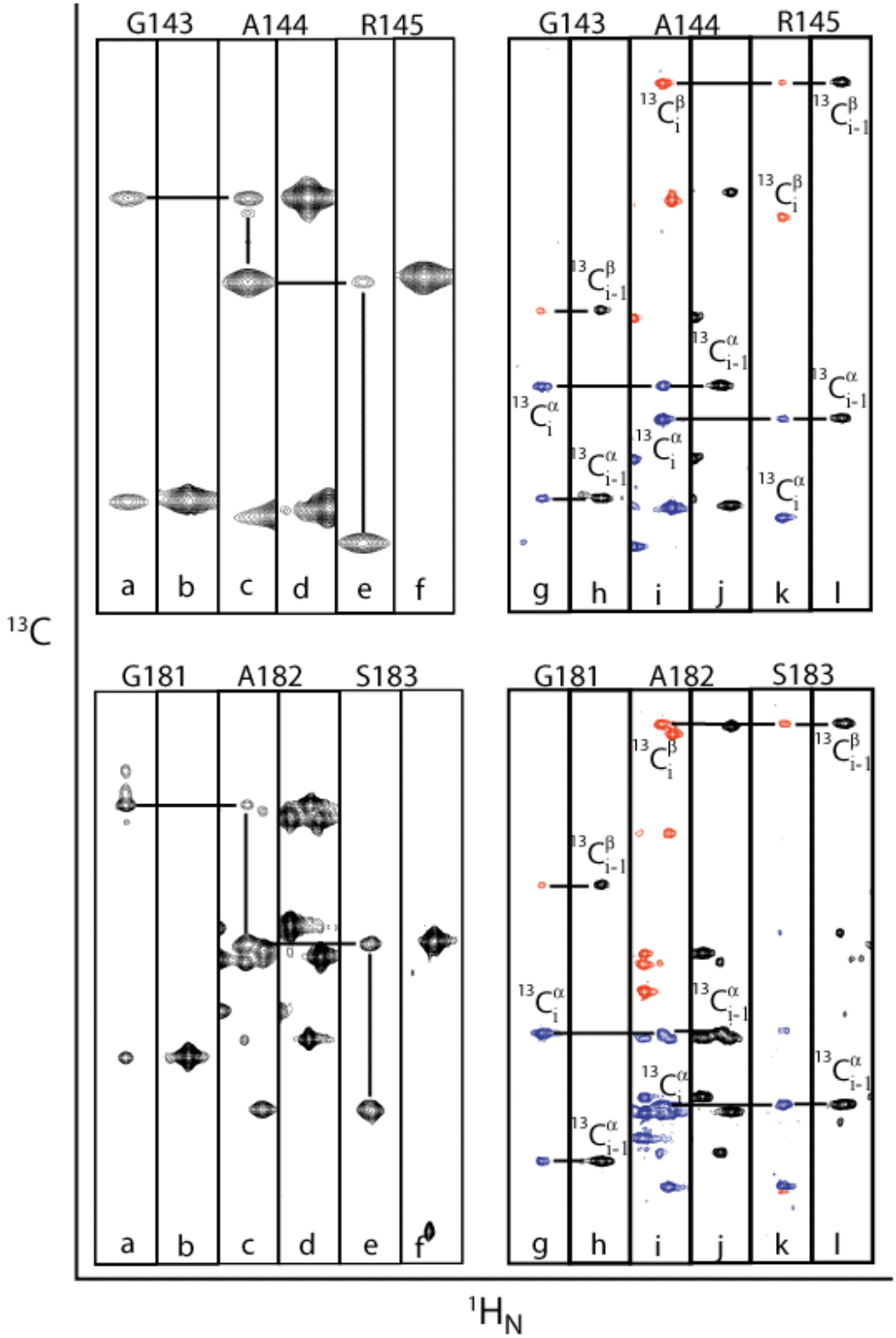

Figure S2. Strip plots taken at $^{1}H_N$ amide resonance frequencies corresponding to residues G143, A144, R145, G181, A182, and S183. The panels shown are sections of HNCA (a, c, e), HN(CO)CA (b, d, f), HNCACB (g, i, k) and CBCA(CO)NH (h, k, l) spectra collected with samples of *pa*-HO-N_3. Straight lines connect resonances exhibiting sequential intra- ($^{13}C_i$) and/or inter-residue ($^{13}C_{i-1}$) correlations with the corresponding amide $^{1}H_N$. Cross-peaks in HNCACB spectra shown in blue were phased positive ($^{13}C^{\alpha}$s) and exhibit a 180° phase difference relative to those shown in red ($^{13}C^{\beta}$s).

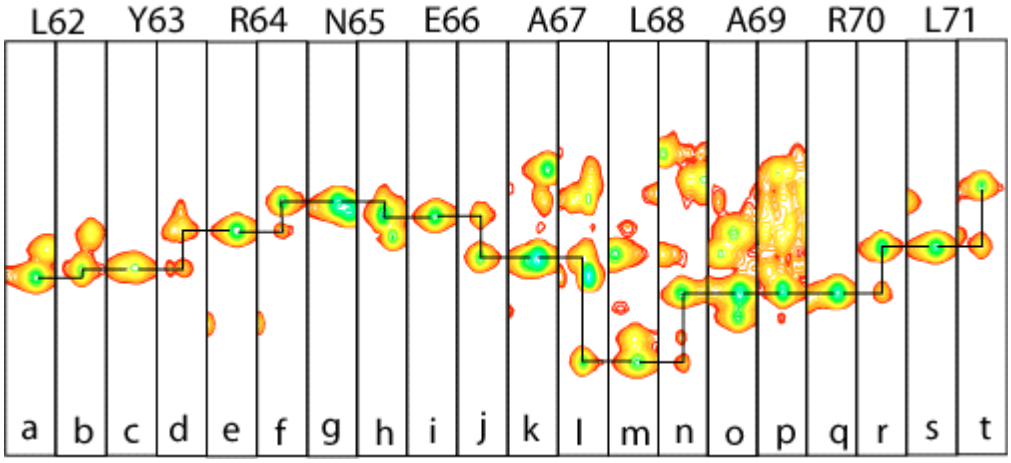

Figure S3. Strip plots taken at the $^{1}H_{N}$ amide chemical shifts (horizontal axis) of residues L62 to L71. The panels shown are sections of HNCO (a, c, e, g, i, k, m, o, q, s) and (HCA)CO(CA)NH (b, d, f, h, j, l, n, p, r, t) spectra collected with samples of *pa*-HO-N_3. ^{13}CO chemical shifts are plotted on the vertical axis. Vertical straight lines in (HCA)CO(CA)NH panels connect pairs of ^{13}CO cross-peaks exhibiting intra- and inter-residue correlations between the ^{13}CO and the amide $^{1}H_{N}$ nucleus. Horizontal straight lines connecting cross-peaks across contiguous panels indicate inter-residue correlations between a $^{1}H_{N}$ resonance and the ^{13}CO resonance of the residue preceding it.

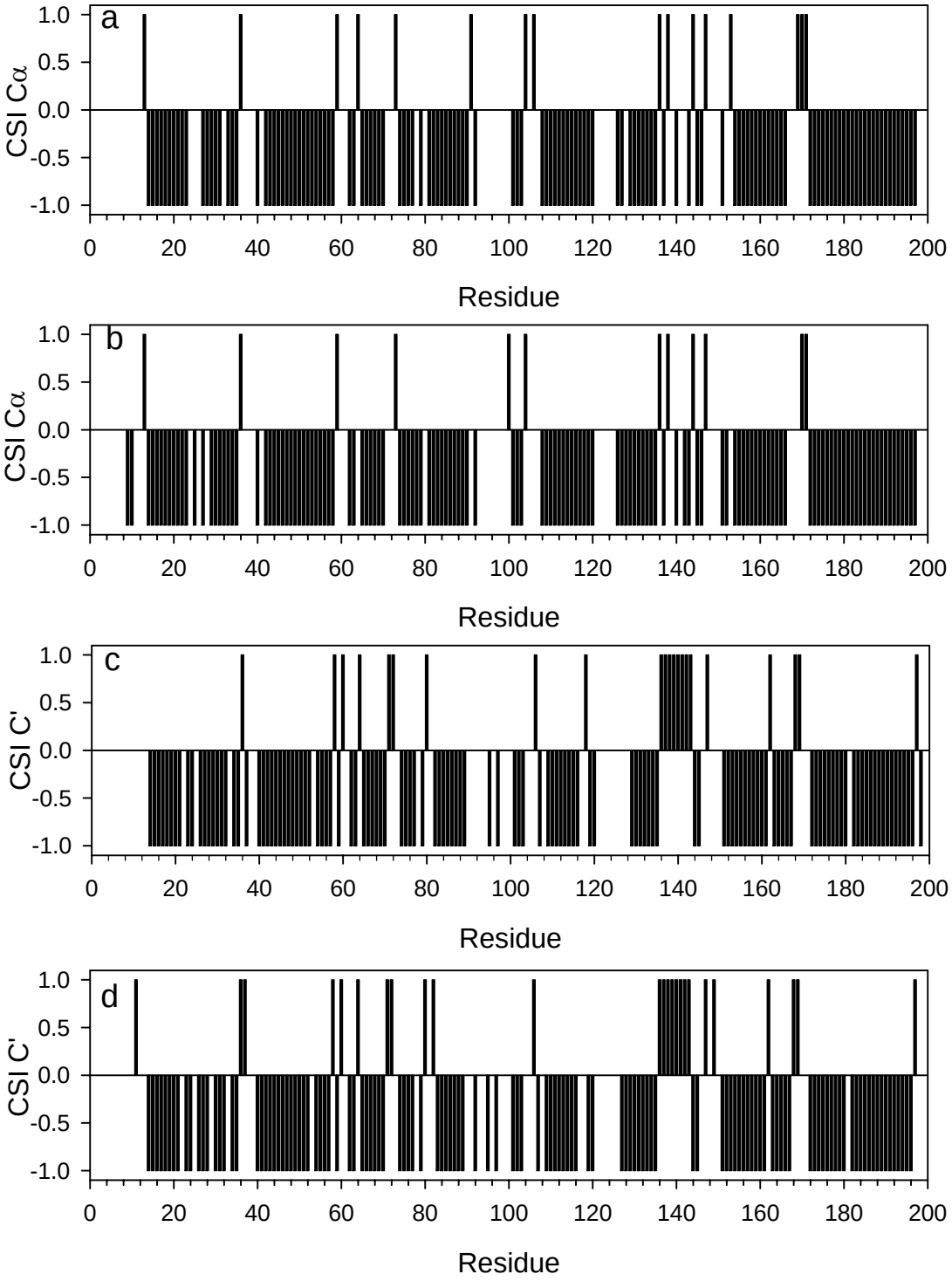

Figure S4. Chemical shift index (CSI) of azide- (a and c) and cyanide-inhibited (b and d) *pa*-HO. CSI values shown in panels (a) and (b) were determined using $^{13}C^{\alpha}$ chemical shifts, whereas those plotted in panels (c) and (d) were calculated using ^{13}CO shifts.

Table S1. Backbone assignments for *pa*-HO-N_3 and *pa*-HO-CN.

	pa-HO-N_3					*pa*-HO-CN				
Residue	$^{1}H_N$	$^{15}N_H$	$^{13}C^{\alpha}$	$^{13}C^{\beta}$	^{13}CO	$^{1}H_N$	$^{15}N_H$	$^{13}C^{\alpha}$	$^{13}C^{\beta}$	^{13}CO
Met1										
Asp2										
Thr3	7.80	119.17								
Leu4										
Ala5	8.20	126.16				8.10	125.65			
Pro6										
Glu7										
Ser8	8.35	117.05								
Thr9						7.87	120.68	62.60	69.94	
Arg10			56.87	30.39		8.13	122.54	57.18	30.68	
Gln11	8.34	120.95	55.81	29.54		8.34	120.75	56.13	29.75	175.52
Asn12	8.37	119.32	53.11	38.73	174.92	8.32	119.07	53.36	39.01	174.90
Leu13	7.96	121.29	54.34	42.59	177.52	7.99	121.25	54.63	42.87	177.53
Arg14	8.83	128.01	60.97	28.64	178.22	8.82	128.09	61.30	28.88	178.21
Ser15	11.55	117.66	60.46	61.49	177.00	11.52	117.61	60.69	61.74	176.97
Gln16	6.76	121.96	58.32	28.36	178.74	6.70	121.85	58.60	28.60	178.67
Arg17	8.11	121.53	60.34	30.14	179.92	8.19	121.65	60.63	30.44	179.86
Leu18	8.88	118.86	57.88	40.36	179.52	8.89	118.84	58.03	40.22	179.73
Asn19	8.16	120.87	57.01	39.21	177.54	8.02	120.71	57.43	39.32	177.45
Leu20	8.10	119.82	58.61	41.78	180.81	8.04	119.81	58.88	42.26	180.86
Leu21	8.32	119.35	57.82	42.82	179.01	8.39	119.39	58.18	43.12	179.08
Thr22	8.08	105.93	62.51	69.97	175.64	8.13	105.93	62.88	70.50	175.67
Asn23	8.24	124.29	59.61	40.26	178.40	8.24	124.31	59.91	40.55	178.31
Glu24	9.86	120.00			177.43	9.83	120.02			177.73
Pro25			66.79	30.41	179.93			67.05	30.78	179.80
His26	10.37	121.28	76.82	40.46	180.65	10.36	120.44	82.52	24.64	179.49
Gln27	10.88	123.45	61.28	29.72	180.92	10.63	123.13	61.35	29.88	180.48
Arg28	9.16	120.79	59.91	30.37	179.66	8.85	120.43	56.95	30.51	179.19
Leu29	9.10	123.08	56.82	40.30	177.87	8.53	122.51	55.51	42.84	176.97
Glu30	9.74	121.21	60.04	28.32	178.45	8.47	120.05	59.01	27.77	177.66
Ser31	7.67	113.48	61.57	62.80	176.65	7.15	112.88	61.61	62.89	176.37
Leu32	7.93	125.08	56.36	42.11	180.01	7.44	124.55	57.67	41.64	179.62
Val33	8.45	118.89	67.10	30.63	177.25	7.70	118.81	66.90	30.22	177.04
Lys34	7.42	116.60	59.97	31.61	180.52	7.07	116.32	60.15	31.75	180.31
Ser35	7.78	115.34	61.06	62.91	174.75	7.52	115.03	61.22	63.08	174.64
Lys36	7.02	119.36	54.09	29.76	175.12	6.86	119.22	54.26	30.01	175.11
Glu37	7.45	110.96			179.02	7.31	110.76			175.02
Pro38			64.88	31.60	173.57			65.08	31.85	173.54
Phe39	7.87	108.36	57.44	37.83	175.84	7.82	108.49	57.59	38.13	175.88
Ala40	7.76	120.81	54.44	19.64	177.86	7.70	120.66	54.70	19.96	177.82
Ser41	7.44	104.51			174.32	7.42	104.67			174.29
Arg42			61.11	30.31	177.34			61.42	30.62	177.33
Asp43	8.19	118.06	57.59	40.83	178.13	8.18	117.96	57.82	41.11	178.10
Asn44	7.98	120.85	55.91	37.00	177.44	7.94	120.72	56.20	37.24	177.39
Phe45	8.57	123.85	63.27	39.06	178.40	8.53	123.84	63.38	39.33	178.42
Ala46	8.86	120.70	55.34	17.63	178.91	8.82	120.68	55.54	17.94	178.83
Arg47	7.04	116.63	59.47	27.50	178.70	6.98	116.51	59.67	27.73	178.62
Phe48	7.56	123.61	59.90	38.73	176.67	7.48	123.60	60.18	38.99	176.66
Val49	8.87	120.94	66.59	30.35	177.65	8.81	121.14	66.86	30.74	177.68
Ala50	8.46	122.02	56.05	17.10	178.38	8.44	121.86	56.25	17.37	178.36
Ala51	7.09	121.07	55.79	16.41	178.35	7.04	121.05	55.96	16.72	178.35
Gln52	7.90	116.34	59.51	28.92	179.72	7.82	116.45	59.97	29.11	179.60
Tyr53	9.47	119.11	62.19	37.65	176.05	9.46	119.14	62.48	37.96	176.20
Leu54	8.29	120.05	58.19	42.43	178.87	8.34	120.11	58.46	42.62	179.03

Phe55	8.44	122.02	60.23	39.55	177.17	8.51	122.35	60.74	40.00	177.31
Gln56	8.38	114.81	58.07	27.20	178.81	8.49	115.11	58.51	27.66	178.93
His57	9.08	121.85	59.25	28.15	178.01	9.09	121.85	59.56	28.37	177.92
Asp58	7.86	122.28	57.73	40.27	175.57	7.94	122.29	58.06	40.69	175.74
Leu59	6.67	112.77	54.09	42.62	177.94	6.79	113.19	54.36	42.92	178.02
Glu60	7.46	124.77			174.09	7.50	124.55			174.26
Pro61			65.12	30.86	178.37			65.47	31.20	178.57
Leu62	7.57	116.03	57.16	40.75	178.13	7.62	116.30	57.56	41.54	178.17
Tyr63	7.76	115.09	62.95	38.83	176.80	7.78	115.10	63.16	39.05	176.80
Arg64	7.32	111.62	55.54	29.72	175.75	7.37	111.85	55.82	30.09	175.83
Asn65	7.20	122.72	55.09	40.51	176.26	7.25	122.79	55.38	40.81	176.30
Glu66	9.09	128.31	59.97	29.73	177.83	9.11	128.34	60.28	30.06	177.87
Ala67	7.89	122.40	55.42	17.83	181.77	7.92	122.34	55.67	18.15	181.71
Leu68	8.40	119.11	57.90	41.67	179.16	8.40	119.12	58.24	42.10	179.15
Ala69	8.36	122.35	54.35	18.06	179.12	8.38	122.28	54.66	18.37	179.14
Arg70	7.25	114.68	58.29	30.29	177.48	7.28	114.72	58.59	30.60	177.50
Leu71	7.07	118.37	56.05	43.79	175.25	7.09	118.44	56.34	44.13	175.30
Phe72	7.95	115.72			171.93	7.97	115.67			172.09
Pro73			58.64	29.01	178.31			58.89	29.36	178.23
Gly74	9.01	115.93	46.13		176.42	8.98	115.79	46.40		176.42
Leu75	8.00	123.21	59.21	41.56	178.13	7.98	123.20	59.44	41.88	178.14
Ala76	8.82	117.60	55.81	17.88	180.78	8.80	117.65	56.05	18.24	180.67
Ser77	7.92	111.65	60.11	63.61	175.02	7.92	111.62	60.38	63.90	175.07
Arg78	8.18	120.02	56.80	30.27	176.41	8.18	119.95	57.07	30.67	176.39
Ala79	6.73	123.01	56.48	19.19	178.13	6.79	123.05	53.44	20.14	178.16
Arg80	7.69	117.17	55.73	32.82	175.76	7.82	117.45	56.08	33.01	175.86
Asp81	8.96	120.72	58.49	38.62	177.05	8.98	120.61	58.71	39.09	177.12
Asp82	8.29	120.05	57.76	40.09	179.16	8.30	119.81	58.04	40.44	175.69
Ala83	8.21	123.90	55.33	17.84	178.05	8.16	123.71	55.64	18.22	178.08
Ala84	8.19	117.30	55.24	17.23	178.44	8.18	117.27	55.41	17.53	178.46
Arg85	8.42	118.36	60.21	29.63	178.86	8.43	118.27	60.48	30.22	178.85
Ala86	8.00	123.21	55.43	17.21	179.98	7.98	123.20	55.63	17.51	179.98
Asp87	8.43	122.25	58.54	41.25	178.95	8.38	122.22	58.80	41.53	178.96
Leu88	7.91	119.11	58.70	40.38	178.77	7.89	119.04	58.97	40.59	178.77
Ala89	7.52	120.75	55.06	17.45	182.38	7.51	120.70	55.27	17.75	182.37
Asp90	8.29	121.49	57.52	40.09	177.52	8.28	121.49	57.73	40.39	177.54
Leu91	7.57	116.03	54.93	42.45	176.88	7.58	115.96	55.16	42.70	176.91
Gly92	8.05	109.25	46.21		174.05	8.03	109.24	46.51		176.12
His93	8.20	122.71				8.21	122.81			174.97
Pro94			62.35	32.78	177.01			62.58	32.98	177.00
Val95	8.89	124.25			178.22	8.86	124.06			178.22
Pro96			62.20	31.99	175.43			62.49	32.26	175.48
Glu97	8.42	119.82	56.56	30.38	176.94	8.43	119.88	56.90	30.67	176.95
Gly98	8.45	111.12	44.69		173.29	8.46	111.11	45.00		173.30
Asp99	8.66	119.95	52.97	43.15	177.15	8.67	120.00	53.30	43.45	177.17
Gln100	8.74	117.86	55.09	28.62	176.63	8.75	117.79	55.41	28.96	176.67
Ser101	8.80	116.99	62.21	63.33	175.32	8.82	117.01	62.63	63.67	175.38
Val102	8.26	122.86	64.23	32.14	178.23	8.31	122.82	64.52	32.72	178.20
Arg103	8.27	121.45	58.98	31.12	177.99	8.33	121.58	59.26	31.53	178.04
Glu104	7.75	114.31	55.50	28.89	176.03	7.79	114.43	55.95	29.21	176.03
Ala105	7.15	122.78	52.88	18.54	177.01	7.20	122.88	53.19	18.90	177.05
Asp106	8.35	120.71	53.33	39.51	175.39	8.39	120.81	53.64	39.89	175.44
Leu107	7.69	121.45	55.11	43.05	177.69	7.74	121.59	55.46	43.35	177.73
Ser108	8.46	118.91	58.30	65.14	173.98	8.50	118.96	58.62	65.45	174.07
Leu109	8.51	123.13	59.46	41.41	178.30	8.54	123.23	59.75	41.71	178.30
Ala110	8.26	116.93	55.74	19.95	178.61	8.30	116.92	56.08	20.28	178.73
Glu111	7.37	115.51	59.43	31.14	179.88	7.43	115.46	59.81	31.53	179.99
Ala112	8.58	120.83	55.38	19.13	179.32	8.65	120.94	55.76	19.40	179.44
Leu113	8.04	115.68	58.31	41.47	179.08	8.11	115.75	58.66	41.78	179.23
Gly114	7.55	104.14	47.85		175.33	7.67	104.28	48.19		175.58
Trp115	7.38	121.40	62.03	27.94	178.60	7.54	121.63	62.59	28.39	178.93

Leu116	8.29	117.20	57.67	42.02	177.99	8.49	117.62	58.01	42.60	178.25
Phe117	8.37	119.39	62.21	38.71	175.30	8.53	119.54	62.77	39.22	175.81
Val118	6.76	117.66	64.40	29.76	176.04	7.18	118.12	65.62	31.10	177.10
Ser119	7.39	111.17	61.12	63.36	179.10	7.99	112.00	61.87	63.87	179.53
Glu120	8.71	116.94	58.60	28.03	179.34	9.05	117.54	58.92	28.59	179.42
Gly121	7.35	111.69				7.75	111.94	45.39		173.13
Ser122						6.51	114.35			
Lys123	10.18	130.05								
Leu124	9.50	120.60				8.20	120.10			
Gly125		132.70				9.10	123.00			
Ala126	14.80	126.90	59.15	22.01		13.20	124.10	58.53	21.95	
Ala127	8.61	119.82	55.32	17.89		8.49	119.53	56.56	19.28	180.51
Phe128	8.20	117.29				8.21	117.68	60.63	38.77	179.28
Leu129	8.14	119.98	58.25	44.31	178.29	8.60	120.45	58.87	44.56	178.45
Phe130	9.86	119.76	62.70	39.30	177.54	10.04	120.39	62.98	39.77	177.59
Lys131	7.12	116.78	59.08	32.32	179.99	7.40	117.03	59.51	32.67	179.98
Lys132	7.33	119.69	59.83	30.59	178.77	7.41	119.57	60.06	30.85	178.86
Ala133	8.06	122.09	54.38	16.84	178.51	8.14	122.19	54.72	17.26	178.67
Ala134	7.23	120.71	54.84	17.71	181.40	7.39	120.86	55.12	17.99	181.46
Ala135	7.46	121.10	54.44	18.52	178.86	7.44	121.03	54.73	18.79	178.85
Leu136	7.43	116.77	53.70	42.29	175.31	7.46	116.92	54.09	42.53	175.39
Glu137	8.15	115.25	57.49	26.43	173.69	8.17	115.27	57.79	26.71	173.80
Leu138	6.85	116.37	53.00	42.45	176.28	6.83	116.44	53.31	42.74	176.24
Asp139	9.34	121.54	54.32	40.82	175.67	9.33	121.21	54.61	41.19	175.66
Glu140	10.58	116.82	58.73	28.51	174.76	10.52	116.79	59.03	28.84	174.80
Asn141	8.86	116.76	53.06	41.13	174.56	8.86	116.63	53.34	41.42	174.56
Phe142	7.89	122.40	58.52	40.42	175.17	7.89	122.56	58.82	40.64	175.15
Gly143	9.72	119.09	47.67		170.91	9.72	119.12	47.93		170.94
Ala144	7.53	118.84	51.02	18.62	179.12	7.51	118.82	51.35	18.91	179.08
Arg145	11.14	125.24	60.38	31.48	183.78	11.16	125.29	60.63	31.66	183.75
His146	11.22	116.09	59.54	27.47	174.75	11.25	116.25	59.88	27.71	174.95
Leu147	7.70	120.35	54.35	44.61	175.87	7.65	120.44	54.62	44.91	175.81
Ala148	7.59	123.05	52.17	20.56	176.88	7.57	123.08	52.48	20.76	176.91
Glu149	8.39	122.34				8.39	122.54			174.68
Pro150										
Glu151			63.86	31.39	179.47			64.19	31.70	179.46
Gly152	9.14	113.91	45.51		174.78	9.13	113.78	45.77		174.84
Gly153	8.20	108.08	44.29		175.88	8.16	107.98	44.56		175.71
Arg154	9.61	126.36	59.79	31.59	178.25	9.47	125.28	59.86	31.46	178.17
Ala155	8.82	122.70	55.70	17.67	180.67	8.67	122.50	55.86	17.90	180.40
Gln156	9.14	119.10	59.32	27.51	179.19	8.99	118.95	59.43	27.80	179.10
Gly157	7.88	107.35	47.27		177.11	7.76	107.15	47.48		176.95
Trp158	7.76	125.41	58.63	30.68	176.77	7.63	125.08	58.95	30.73	176.72
Lys159	8.44	118.37	59.80	32.28	179.63	8.31	118.19	60.04	32.48	179.53
Ser160	8.26	112.72	61.02	62.77	176.46	8.13	112.59	61.24	63.03	176.34
Phe161	7.28	124.06	61.99	39.33	176.57	7.22	123.85	61.99	39.61	176.58
Val162	8.36	117.45	65.90	30.72	176.44	8.34	117.30	66.00	30.88	176.44
Ala163	7.64	119.74	54.94	17.89	181.09	7.56	119.86	55.16	18.17	181.06
Ile164	6.80	116.98	63.90	37.21	178.87	6.77	116.89	63.99	37.52	178.85
Leu165	7.96	121.29	58.45	42.20	178.31	7.94	121.24	58.76	42.52	178.27
Asp166	8.68	116.61	56.88	40.06	178.24	8.67	116.45	57.09	40.27	178.23
Gly167	7.50	106.45	45.07		174.46	7.48	106.51	45.35		174.50
Ile168	6.83	121.07	62.49	39.04	176.04	6.83	121.08	62.79	39.38	176.06
Glu169	8.71	129.50	55.92	29.62	174.53	8.71	129.48	56.21	29.93	174.58
Leu170	7.89	124.80	53.10	44.14	177.11	7.90	124.81	53.42	44.45	177.16
Asn171	9.49	121.35	51.49	38.14	175.33	9.51	121.37	51.79	38.44	175.40
Glu172	8.46	116.91	60.76	29.55	179.10	8.47	116.91	61.07	29.86	179.13
Glu173	8.09	121.00	59.31	29.00	179.23	8.10	121.03	59.55	29.30	179.30
Glu174	8.58	120.42	59.01	31.18	178.69	8.60	120.45	59.34	31.52	178.73
Glu175	8.65	119.49	59.16	29.05	180.59	8.68	119.61	59.49	29.40	180.63
Arg176	7.45	118.98	59.83	29.85	179.77	7.48	119.04	59.88	30.11	179.81

Leu177	8.03	122.52	57.84	40.13	178.50	8.07	122.57	57.98	42.52	178.59
Ala178	8.19	123.62	55.66	16.37	179.32	8.26	124.00	55.99	16.73	179.44
Ala179	7.21	118.39	54.81	18.06	179.66	7.28	118.49	55.33	18.48	179.81
Lys180	8.11	121.53	59.61	32.95	178.07	8.19	121.65	59.99	33.32	178.21
Gly181	8.77	106.57	47.22		173.64	8.87	106.71	47.68		173.85
Ala182	7.49	121.05	54.20	17.51	178.95	7.64	121.23	54.73	18.05	179.25
Ser183	7.76	112.49	52.87	62.92	177.46	7.92	112.69	53.23	63.28	177.59
Asp184	9.15	122.41	56.99	39.25	178.46	9.33	122.72	57.38	39.58	178.66
Ala185	7.55	125.46	54.50	17.83	179.12	7.77	125.66	55.08	18.43	179.46
Phe186	7.09	114.95	63.89	39.38	178.80	7.43	115.46	64.29	39.96	178.94
Asn187	7.55	117.29	55.88	37.62	177.46	7.74	117.56	56.25	37.98	177.57
Arg188	8.45	121.40	57.62	30.67	177.26	8.59	121.49	63.88	30.99	177.42
Phe189	7.91	119.11	62.64	38.03	177.26	8.08	119.28	62.90	38.27	177.34
Gly190	7.55	102.64	47.72		175.13	7.56	102.75	47.87		175.11
Asp191	7.63	121.63	57.44	40.48	179.72	7.62	121.67	57.66	40.87	179.53
Leu192	8.16	120.87	57.90	41.75	178.07	8.18	120.81	58.06	41.99	178.06
Leu193	8.13	119.22	57.13	42.43	178.56	8.06	119.18	57.37	42.56	178.50
Glu194	7.64	115.14	58.56	28.84	179.69	7.56	115.21	58.82	29.08	179.57
Arg195	7.69	118.10	59.33	30.25	179.88	7.62	117.95	59.49	30.49	179.81
Thr196	8.73	110.79	65.10	67.97	177.42	8.71	110.87	65.27	68.21	177.40
Phe197	7.71	119.96	60.33	38.42	174.16	7.67	119.92	60.50	38.60	174.12
Ala198	7.05	129.37			182.82	7.00	129.32			