

Supporting Information.

Table 1. NMR experimental parameters.^{a)}

NMR experiment	Field (MHz)	F ₁ (ni; sw; at)	F ₂ (ni; sw; at)	F ₃ (ni; sw; at)	F ₄ (ni; sw; at)	Scans; d1; total time
4D HNCACO ^{b)}	800	CA: 24*; 3550 Hz; 6.5 ms	CO: 14*; 2011 Hz; 6.7 ms	¹⁵ N: 40*; 2268 Hz; 17.2 ms	HN: 818*; 12775.5 Hz; 64.0 ms	4; 1.55 s; 205 hrs.
4D HNCOCA ^{b)}	600	CO: 12*; 1506 Hz; 7.3 ms	CA: 22*; 2662.5 Hz; 8.1 ms	¹⁵ N: 40*; 1700 Hz; 22.9 ms	HN: 612*; 9564.8 Hz; 64.0 ms	4; 1.60 s; 166 hrs.
4D HNCO _{i-1} CA _i ^{b)}	800	CO: 14*; 2011 Hz; 6.7 ms	CA: 22*; 3550 Hz; 6.1 ms	¹⁵ N: 40*; 2268 Hz; 17.2 ms	HN: 818*; 12775.5 Hz; 64.0 ms	4; 1.56 s; 187 hrs.
4D ¹⁵ N, ¹⁵ N-NOESY ^{c)}	800	¹⁵ N: 20*; 2268 Hz; 8.6 ms	HN: 20*; 3600 Hz; 5.3 ms	¹⁵ N: 32*; 2268 Hz; 13.9 ms	HN: 817*; 12775.5 Hz; 64.0 ms	4; 1.40 s; 183 hrs.
3D HN(CO)CACB ^{d,g)}	600	CACB: 35*; 7380 Hz; 4.7 ms	¹⁵ N: 54*; 1700 Hz; 31.2 ms	HN: 576*; 9000.9 Hz; 64.0 ms		32; 1.52 s; 109 hrs.
3D HNCACB ^{d,g)}	800	CACB: 40*; 7803 Hz; 5.1 ms	¹⁵ N: 64*; 2268 Hz; 27.8 ms	HN: 818*; 12775.5 Hz; 64.0 ms		32; 1.56 s; 157 hrs.
3D HN(CA)CO ^{e,g)}	800	CO: 20*; 2011 Hz; 9.7 ms	¹⁵ N: 64*; 2268 Hz; 27.8 ms	HN: 818*; 12775.5 Hz; 64.0 ms		40; 1.46 s; 89 hrs.
3D HNCO ^{f,g)}	600; 800	CO: 28*; 2011 Hz; 13.7 ms	¹⁵ N: 64*; 2268 Hz; 27.8 ms	HN: 818*; 12775.5 Hz; 64.0 ms		8; 1.8 s; 26 hrs.

^{a)}For each dimension of every experiment, the following parameters are listed: type of nucleus evolved, total number of acquired points, ni, (* - complex points), sweep width in Hz, and maximum acquisition time (ms). In addition, the spectrometer field, the number of scans/FID, relaxation delay (d1) and the total experimental acquisition time are listed for each experiment.

^{b)}4D TROSY-HNCACO, TROSY-HNCOCA and TROSY-HNCO_{i-1}CA_i were recorded as described earlier^{1, 2} ^{c)}4D ¹⁵N, ¹⁵N-NOESY^{3, 4} spectrum (mixing time of 90 ms) was recorded with the selection of the TROSY component in the F₃ (¹⁵N) / F₄ (¹HN) dimensions. ^{d)}Both 3D TROSY-HN(CO)CACB and TROSY-HNCACB experiments were recorded with non-constant-time ¹³C^β evolution periods¹. The ¹³C^α-¹³C^β transfer delays were optimized for better sensitivity of ¹³C^β peaks

and were set to 10 ms. This led to the appearance of typically weak $^{13}\text{C}^{\alpha}$ correlations in the addition to the $^{13}\text{C}^{\beta}$ correlations. Different spectral widths (in ppm) were used in F_1 dimensions of HNCACB and HN(CO)CACB in order to resolve ambiguities associated primarily with the folding of Ala, Thr and Ser C^{β} resonances. ^{e)}A $^{13}\text{C}^{\alpha}$ - ^{13}CO transfer period of 5.4 ms was used. ^{f)}3D TROSY-HNCO experiment was recorded on both 600 and 800 MHz spectrometers. The parameters are listed for the 800 MHz experiment. On average, a sensitivity improvement of 33 % was observed in the 800 MHz TROSY-HNCO spectrum compared to the 600 MHz TROSY-HNCO recorded with the same total acquisition time. ^{g)}Experiment was recorded with shared constant time evolution in F_2 (^{15}N) dimension.

Table 2. Backbone and C^β chemical shifts of Malate synthase G at pH 7.1 and 37 °C.^{a)}

Res.	HN	N	C ^α	CO	C ^β
M1	****	*****	*****	*****	*****
A2	****	*****	*****	*****	*****
Q3	****	*****	55.65	175.93	28.36
T4	8.27	114.32	59.60	173.24	71.44
I5	8.94	121.58	58.56	175.41	40.13
T6	8.41	121.58	60.93	174.12	68.95
Q7	8.51	127.48	54.68	174.45	29.43
S8	****	*****	60.02	174.53	*****
R9	8.31	123.00	56.24	175.87	29.91
L10	7.99	117.23	53.17	176.22	42.86
R11	8.56	121.84	54.79	175.68	31.34
I12	9.11	124.40	59.85	175.60	41.32
D13	8.90	127.99	56.24	176.54	43.10
A14	8.78	130.11	55.50	179.91	17.68
N15	8.25	118.21	55.28	178.49	36.27
F16	9.46	125.89	62.25	176.07	39.26
K17	8.91	120.19	59.53	177.16	31.73
R18	7.55	117.00	59.26	177.59	28.86
F19	7.72	120.02	59.96	177.32	37.47
V20	8.08	120.80	66.38	177.65	31.01
D21	8.82	119.59	57.13	178.28	39.62
E22	8.67	113.73	56.81	177.65	29.58
E23	7.74	116.23	57.22	176.69	29.46
V24	6.99	117.35	64.40	177.38	31.01
L25	8.44	118.21	58.17	177.27	38.54
P26		*****	67.33	178.85	29.46
G27	7.97	104.72	45.90	174.97	
T28	7.68	109.23	62.30	176.09	70.53
G29	7.34	109.07	44.92	173.75	
L30	7.70	121.75	54.09	176.18	40.81
D31	8.07	121.92	53.33	177.02	42.01
A32	8.76	131.40	55.28	178.28	17.56
A33	8.11	120.02	55.01	181.41	16.48
A34	8.07	121.83	54.25	178.87	17.08
F35	8.23	121.06	60.78	177.48	37.83
W36	8.44	119.33	60.02	179.01	28.74
R37	8.02	121.75	59.15	178.74	28.74
N38	8.65	119.33	55.39	178.11	37.23
F39	8.78	125.20	57.35	177.81	37.11
D40	8.37	120.71	57.62	179.04	41.65
E41	7.91	119.76	59.47	178.38	28.62
I42	8.13	119.59	66.19	177.78	36.75
V43	8.44	120.37	67.28	177.32	30.65

H44	8.25	115.54	61.57	177.10	27.07
D45	8.50	117.78	55.99	178.57	40.00
L46	8.51	116.92	56.26	178.41	41.05
A47	8.82	123.99	57.08	176.56	15.29
P48		*****	65.97	179.72	29.91
E49	6.71	118.94	58.34	177.84	28.25
N50	7.95	120.30	54.73	179.37	39.77
R51	8.32	119.96	60.12	179.37	29.08
Q52	7.84	122.18	58.35	179.10	26.82
L53	7.95	120.30	57.48	180.58	39.65
L54	7.31	119.88	57.37	179.23	36.33
A55	7.72	123.69	54.31	181.08	16.60
E56	8.01	121.49	57.71	178.71	28.02
R57	7.47	117.44	59.31	179.88	29.46
D58	7.20	120.45	56.92	178.74	38.90
R59	8.03	123.73	58.98	179.56	29.22
I60	8.31	121.49	64.69	177.48	36.75
Q61	8.37	119.59	57.46	178.03	27.78
A62	7.95	121.32	54.80	180.56	16.48
A63	7.58	121.32	54.41	181.14	18.52
L64	8.61	123.04	58.66	178.63	41.05
D65	9.10	119.50	56.43	178.06	39.62
E66	7.49	117.87	58.60	178.74	28.38
W67	8.22	122.87	63.01	179.86	29.46
H68	9.05	117.69	60.51	175.60	27.30
R69	8.14	116.66	58.44	179.12	29.93
S70	7.47	113.38	59.83	173.05	62.58
N71	7.20	119.59	50.31	180.67	37.95
P72		*****	63.68	177.11	32.09
G73	8.64	107.01	43.65	171.06	
P74		*****	62.49	176.68	30.98
V75	8.59	124.06	62.60	176.14	29.91
K76	8.32	130.38	56.94	176.38	31.69
D77	7.75	119.62	51.50	177.30	39.53
K78	****	*****	58.56	178.10	30.39
A79	8.23	122.83	55.00	180.60	16.78
A80	7.87	122.78	53.98	181.14	17.25
Y81	7.78	120.73	58.45	177.00	38.47
K82	8.57	117.78	60.50	178.27	30.98
S83	8.05	114.09	61.70	176.54	*****
F84	7.68	123.89	59.80	176.54	36.92
L85	8.10	118.25	56.51	180.77	40.13
R86	8.48	122.61	58.77	180.10	28.74
E87	8.11	123.99	58.71	178.28	28.14
L88	7.65	117.87	54.41	175.90	42.25
G89	7.38	103.75	43.56	173.42	
Y90	7.92	120.89	59.15	175.68	40.22
L91	6.68	117.44	52.67	175.17	42.85
V92	8.23	119.59	57.62	174.08	30.65
P93		*****	62.81	176.79	30.53
Q94	8.71	123.25	51.62	173.88	27.34
P95		*****	61.47	176.09	31.34
E96	8.45	120.22	57.43	176.25	29.08
R97	7.48	115.95	54.84	174.42	31.34

V98	8.23	124.23	61.25	173.26	34.66
T99	8.18	120.22	59.80	173.59	69.78
V100	7.98	126.28	62.28	175.33	31.57
E101	8.00	128.59	54.68	174.74	30.50
T102	7.44	113.56	58.34	174.45	70.97
T103	8.05	111.93	59.21	174.10	70.97
G104	****	*****	46.14	176.87	
I105	8.35	126.10	58.72	175.87	34.31
D106	7.65	127.09	55.49	177.32	42.62
S107	9.34	118.79	60.28	176.44	62.11
E108	9.97	125.23	60.66	176.19	28.36
I109	7.19	112.77	61.63	177.16	37.51
T110	7.55	108.47	63.15	177.57	68.73
S111	8.41	114.42	58.14	173.23	64.25
Q112	7.00	118.56	54.03	172.09	33.76
A113	6.66	119.76	51.75	175.30	19.95
G114	7.65	108.04	43.84	168.57	
P115		*****	62.58	174.10	33.35
Q116	8.01	123.25	53.57	174.26	33.84
L117	7.39	126.35	53.07	175.66	43.28
V118	7.45	120.95	61.32	174.65	32.13
V119	8.37	119.89	55.47	171.27	34.02
P120		*****	61.36	177.97	31.81
A121	8.57	125.50	52.63	175.36	16.42
M122	6.05	110.99	55.49	172.89	33.83
N123	7.01	117.09	51.23	173.40	38.94
A124	****	*****	*****	*****	*****
R125	****	*****	59.26	178.43	28.48
Y126	7.86	117.34	58.02	179.34	35.61
A127	8.33	122.53	55.16	178.10	16.54
L128	8.35	119.19	57.64	178.05	41.08
N129	7.90	115.52	54.68	177.86	36.68
A130	7.92	121.86	53.76	178.72	19.51
A131	8.24	120.22	54.30	179.66	16.89
N132	7.74	113.56	52.36	176.38	37.63
A133	7.59	122.87	52.15	176.25	16.89
R134	6.54	120.90	56.24	172.65	30.39
W135	6.96	115.44	53.92	175.60	30.27
G136	8.79	110.31	43.98	172.00	
S137	8.61	115.58	57.68	177.51	60.90
L138	9.81	135.61	55.83	178.11	41.29
Y139	7.16	118.30	57.19	178.11	34.12
D140	8.43	120.63	56.92	179.20	40.10
A141	7.52	120.89	54.31	179.26	17.80
L142	7.95	116.14	56.05	179.99	42.49
Y143	8.63	120.37	61.92	178.74	37.71
G144	7.70	104.59	45.12	172.96	
S145	7.23	116.14	57.22	172.48	65.63
D146	8.51	116.75	52.56	176.64	38.54
I147	7.33	119.85	64.26	176.07	36.28
I148	6.35	118.56	55.50	174.49	36.27
P149		*****	63.09	176.61	31.25
Q150	8.57	123.30	54.69	175.41	28.26
E151	8.40	125.63	55.56	176.26	29.46

G152	8.19	110.97	44.33	173.34	
A153	8.04	123.82	51.53	177.54	18.28
M154	8.32	121.23	55.04	176.31	31.85
V155	8.24	122.31	61.02	175.90	31.97
S156	8.23	118.81	57.95	177.27	62.81
G157	****	*****	*****	*****	
Y158	****	*****	58.10	173.48	37.93
D159	7.95	129.56	49.27	174.34	41.71
P160		*****	63.79	178.72	31.10
Q161	8.00	119.02	58.51	178.40	27.18
R162	7.24	122.70	58.45	179.37	27.53
G163	8.80	107.32	47.00	175.47	
E164	8.12	120.39	59.15	179.34	28.36
Q165	7.32	118.34	58.18	179.50	28.84
V166	7.90	123.29	66.19	176.54	30.39
I167	8.34	120.27	65.24	179.88	38.11
A168	8.06	122.35	54.63	179.72	17.37
W169	8.01	122.44	61.47	180.44	30.15
V170	8.36	119.02	66.81	177.32	30.39
R171	8.23	119.88	58.72	177.65	30.62
R172	7.39	117.48	58.88	178.16	28.25
F173	7.51	121.73	60.34	177.65	37.51
L174	8.39	122.27	57.48	178.10	39.30
D175	7.78	118.34	57.16	177.84	39.65
E176	7.44	116.46	57.70	178.56	29.43
S177	7.80	113.73	60.39	173.67	63.77
L178	8.40	123.64	52.79	172.81	40.96
P179		*****	63.40	178.32	30.99
L180	8.57	119.88	52.93	178.13	40.25
E181	8.95	122.69	58.75	176.28	28.43
N182	7.33	115.05	52.43	172.54	40.49
G183	7.70	106.04	43.77	172.00	
S184	7.96	112.96	53.92	176.75	63.66
Y185	10.85	129.62	62.28	179.53	37.99
Q186	9.14	120.47	58.45	177.00	27.89
D187	7.97	117.91	53.49	174.69	41.91
V188	6.76	120.56	63.19	175.82	31.57
V189	8.70	116.29	60.34	175.15	32.88
A190	7.23	120.93	51.91	173.78	21.03
F191	8.71	117.78	55.94	174.38	42.37
K192	8.74	117.69	55.01	173.07	35.20
V193	8.44	123.04	61.10	175.96	30.65
V194	8.69	128.73	60.62	175.71	34.00
D195	9.27	130.20	55.18	174.95	38.54
K196	8.59	108.17	57.30	174.46	29.22
Q197	7.75	117.00	53.11	173.67	31.37
L198	7.68	123.47	53.71	175.17	40.10
R199	9.27	127.87	53.00	174.62	29.70
I200	8.37	124.33	60.67	174.24	39.62
Q201	8.66	127.61	54.44	175.14	29.10
L202	8.66	126.49	53.05	179.47	42.25
K203	8.67	121.75	58.33	176.37	31.61
N204	7.86	115.45	52.40	176.07	36.51
G205	8.07	108.21	44.65	174.43	

K206	7.56	121.40	55.07	174.27	32.21
E207	8.16	120.11	53.87	175.79	32.21
T208	9.30	120.37	58.38	171.81	70.41
T209	8.51	112.87	58.82	174.40	71.01
L210	8.42	121.14	55.18	177.21	42.13
R211	8.66	123.56	58.96	176.99	28.86
T212	8.49	114.59	58.55	172.90	68.02
P213		*****	65.03	177.84	31.34
A214	8.14	118.34	53.06	178.13	17.49
Q215	8.19	115.18	57.43	176.68	28.36
F216	7.84	118.00	56.13	173.26	38.23
V217	8.41	125.77	62.01	176.68	32.64
G218	7.66	106.29	46.30	169.75	
Y219	9.81	118.17	56.13	172.78	38.82
R220	8.01	116.12	55.00	176.28	34.31
G221	8.38	109.33	43.84	172.63	
D222	8.44	120.89	53.90	177.48	41.89
A223	8.53	128.04	55.07	177.48	17.08
A224	8.16	115.19	52.19	178.17	17.92
A225	7.67	119.59	50.69	172.36	16.96
P226		*****	63.30	177.41	32.05
T227	8.65	110.14	61.47	175.76	68.35
C228	7.61	119.19	56.13	172.38	29.55
I229	8.66	124.40	58.45	172.51	38.23
L230	9.12	130.13	53.49	174.15	42.86
L231	9.51	129.87	52.95	175.60	44.64
K232	9.24	120.82	54.95	174.47	35.73
N233	8.96	122.70	52.79	172.48	41.55
N234	8.68	124.92	53.23	174.69	35.02
G235	8.53	102.21	45.06	172.19	
L236	7.78	122.70	52.79	176.25	43.81
H237	9.10	119.45	57.75	176.22	30.86
I238	9.20	123.89	60.88	173.02	41.91
E239	9.99	128.25	53.55	175.47	32.52
L240	9.27	125.34	53.28	175.63	40.60
Q241	8.37	123.29	55.49	174.53	28.48
I242	8.40	128.85	58.99	176.22	36.92
D243	8.70	124.66	54.03	176.09	40.96
A244	9.13	129.79	53.01	175.77	16.30
N245	8.42	113.21	51.93	175.93	38.82
G246	7.15	107.92	43.98	173.26	
R247	8.45	121.42	58.61	177.03	28.60
I248	7.66	117.91	62.44	178.83	37.04
G249	9.70	108.77	45.71	176.25	
K250	8.16	120.39	59.26	177.16	30.80
D251	7.12	116.20	53.71	175.58	41.67
D252	7.39	124.92	51.88	177.08	45.59
P253		*****	64.70	175.58	30.74
A254	7.79	116.63	49.78	176.54	18.08
H255	8.14	112.36	55.00	173.43	24.86
I256	7.83	119.36	62.55	175.84	36.09
N257	9.63	130.47	52.79	172.40	42.27
D258	7.60	113.73	52.09	173.59	42.03
V259	7.97	122.61	61.15	173.02	33.00

I260	9.34	130.64	57.86	174.98	37.63
V261	9.26	120.73	58.24	174.31	32.76
E262	7.82	127.31	55.00	176.22	29.55
A263	7.90	130.64	52.09	173.59	19.51
A264	7.19	118.25	49.61	175.60	15.35
I265	7.56	130.64	61.20	174.82	34.31
S266	7.32	108.00	56.51	172.39	65.86
T267	8.74	117.62	61.36	172.32	74.29
I268	9.08	125.26	59.53	173.94	36.56
L269	8.96	128.85	52.79	175.31	39.89
D270	9.35	126.54	54.84	175.60	42.27
C271	****	*****	57.44	173.02	28.31
E272	8.52	123.78	55.34	177.14	26.73
D273	7.89	121.58	57.33	*****	39.76
S274	****	*****	58.94	172.97	63.52
V275	8.00	117.99	59.69	173.18	33.91
A276	8.19	128.35	49.41	174.59	14.69
A277	8.75	127.87	50.55	176.01	19.59
V278	9.40	112.78	59.20	173.99	32.92
D279	7.09	118.90	51.21	174.92	42.01
A280	8.41	118.90	55.20	178.00	17.80
E281	7.88	117.43	59.01	179.09	28.14
D282	8.46	119.68	56.59	177.95	41.05
K283	7.73	115.62	55.61	177.27	27.54
I284	8.36	119.33	65.86	176.31	37.11
L285	6.96	118.56	57.90	179.04	40.22
L286	7.26	118.90	57.95	178.47	41.41
Y287	8.76	117.44	57.46	178.41	36.87
R288	9.17	122.52	60.29	179.64	28.38
N289	7.68	120.89	55.12	177.92	35.67
L290	7.85	119.33	58.17	178.00	40.94
L291	8.74	121.32	57.79	177.95	41.17
G292	8.08	105.62	46.99	177.48	
L293	8.05	123.56	58.17	178.41	40.46
M294	8.32	117.52	55.67	178.41	32.33
Q295	8.30	114.94	56.43	177.10	28.86
G296	7.43	106.47	44.92	174.76	
T297	8.03	109.76	60.56	174.89	69.21
L298	6.57	124.68	56.10	174.46	41.05
Q299	8.07	121.88	53.65	174.40	30.29
E300	8.55	120.97	54.61	174.29	32.09
K301	8.63	126.06	55.07	175.38	32.57
M302	8.74	122.78	53.98	173.72	34.48
E303	8.36	122.61	54.88	175.74	30.41
K304	8.76	126.06	55.07	174.76	34.00
N305	8.29	131.23	54.77	178.68	42.97
G306	8.54	113.38	45.54	174.26	
R307	8.00	121.42	54.68	175.28	29.91
Q308	8.42	122.61	54.84	175.44	28.72
I309	8.76	125.24	59.42	174.77	39.30
V310	8.29	124.66	60.82	175.36	32.41
R311	8.95	129.42	54.29	173.72	30.72
K312	8.23	121.67	53.70	175.98	34.19
L313	8.50	121.50	54.68	177.67	40.96

N314	9.29	123.21	52.15	176.25	38.23
D315	8.26	120.73	53.06	176.30	41.55
D316	8.33	119.36	54.52	174.02	39.53
R317	8.07	118.59	54.57	174.26	33.00
H318	8.05	121.84	54.46	174.15	30.39
Y319	8.71	119.36	55.65	174.23	40.84
T320	8.81	120.19	61.35	173.39	68.26
A321	9.34	128.48	50.99	178.63	18.75
A322	7.26	122.52	55.31	177.51	18.16
D323	7.62	110.88	53.00	177.32	39.26
G324	8.51	110.02	44.54	174.51	
S325	8.03	118.21	58.00	172.03	62.93
E326	8.32	120.37	56.16	176.75	30.17
I327	8.53	120.80	59.42	174.40	41.41
S328	8.19	118.13	55.75	173.26	64.13
L329	9.11	124.68	52.35	176.31	43.33
H330	8.62	123.56	56.48	178.57	29.70
G331	9.08	111.83	45.68	172.14	
R332	6.74	116.75	53.22	175.60	31.97
S333	9.70	120.02	58.66	174.62	64.13
L334	8.55	130.02	56.21	175.00	40.70
L335	9.90	128.90	54.41	176.72	40.46
F336	9.37	125.45	52.89	175.71	40.81
I337	9.06	119.85	60.12	176.31	41.05
R338	8.67	127.52	54.69	176.78	31.13
N339	7.40	126.23	52.19	172.17	42.37
V340	8.84	110.88	62.57	176.97	31.37
G341	****	*****	*****	*****	
H342	****	*****	55.32	176.65	31.39
L343	7.21	117.68	59.07	177.42	42.07
M344	8.83	114.77	54.71	179.21	30.16
T345	8.20	113.35	60.09	172.65	69.06
I346	8.16	120.18	55.84	173.59	42.81
P347		*****	61.63	173.26	27.77
V348	7.67	122.83	62.39	172.11	34.19
I349	5.93	116.12	58.56	172.24	41.91
W350	9.50	127.22	56.62	175.28	33.24
D351	8.51	119.96	51.88	178.13	40.84
S352	9.86	115.26	60.88	176.06	62.35
E353	8.16	121.50	55.16	176.41	29.32
G354	8.23	108.43	44.79	174.63	
N355	8.68	120.82	52.52	176.06	38.11
E356	8.73	123.72	55.81	176.76	30.03
I357	****	*****	*****	*****	*****
P358		*****	*****	*****	*****
E359	****	*****	*****	*****	*****
G360	****	*****	*****	*****	
I361	****	*****	65.62	176.28	36.56
L362	7.29	121.07	58.72	177.32	40.72
D363	9.23	115.86	56.94	179.96	39.65
G364	7.87	110.05	47.38	174.50	
V365	7.95	122.53	66.29	177.35	30.50
M366	8.12	113.64	54.90	178.59	27.65
T367	8.58	115.26	67.52	175.82	*****

G368	8.02	108.00	46.95	172.94	
A369	8.15	122.18	54.57	178.43	15.94
I370	8.03	115.35	64.38	177.81	37.16
A371	8.46	121.42	54.03	179.37	18.80
L372	7.53	119.45	57.64	180.12	39.89
Y373	7.75	115.09	62.71	178.59	36.45
D374	7.57	118.25	56.51	178.88	42.39
L375	7.68	118.94	57.05	178.27	38.94
K376	7.00	115.78	57.75	177.65	32.29
V377	8.01	115.04	63.30	176.57	32.29
Q378	9.17	117.40	56.30	175.28	25.21
K379	7.14	115.52	56.67	175.93	32.05
N380	9.86	119.68	53.66	173.16	37.16
S381	9.43	115.95	56.84	177.15	64.13
R382	9.50	129.62	56.89	177.43	30.74
T383	8.20	109.97	61.06	175.20	67.52
G384	7.83	111.25	45.87	174.26	
S385	8.18	115.62	58.20	170.95	66.22
V386	7.36	121.66	59.85	173.34	33.76
Y387	9.21	127.01	56.26	173.67	38.66
I388	8.40	123.47	59.34	176.39	37.95
V389	9.31	128.39	61.59	174.16	31.37
K390	9.28	129.69	48.54	173.83	31.25
P391		*****	61.99	176.21	32.25
K392	10.08	114.59	57.76	175.47	33.97
M393	8.70	117.77	56.92	177.94	33.48
H394	9.55	127.19	54.73	174.61	31.36
G395	8.48	108.53	44.82	*****	
P396		*****	65.62	178.97	32.05
Q397	8.37	121.42	58.56	180.12	26.23
E398	8.14	121.16	60.12	179.82	28.01
V399	7.45	123.38	65.46	177.94	29.67
A400	8.55	124.66	54.84	180.60	16.18
F401	8.00	119.72	60.77	176.19	38.23
A402	7.37	121.24	54.57	177.41	17.13
N403	8.50	116.89	57.37	177.08	39.18
K404	8.26	124.06	59.42	177.89	31.10
L405	8.22	120.73	57.59	177.54	39.41
F406	8.54	118.94	58.88	177.16	34.66
T407	8.05	118.17	65.97	176.62	68.35
R408	8.18	120.99	55.97	179.99	27.18
I409	8.43	123.38	65.35	176.87	36.92
E410	7.93	118.51	59.10	179.13	26.82
T411	7.87	113.00	65.51	177.38	67.99
M412	7.63	120.54	58.11	176.47	31.21
L413	7.67	117.69	53.60	175.30	40.34
G414	7.43	106.83	45.68	175.49	
M415	8.10	118.38	54.58	175.30	33.94
A416	8.49	124.68	49.68	176.01	15.66
P417		*****	62.92	177.41	30.74
N418	9.09	117.40	55.11	174.12	35.97
T419	7.51	121.42	67.64	173.88	69.54
L420	8.77	117.28	53.49	175.15	38.70
K421	9.31	127.05	52.74	175.15	31.10

M422	8.39	120.05	53.33	176.25	38.94
G423	9.38	114.15	44.09	172.16	
I424	9.10	127.99	60.45	175.28	38.47
M425	6.54	122.32	56.33	175.11	30.41
D426	****	*****	*****	*****	*****
E427	****	*****	*****	*****	*****
E428	****	*****	*****	*****	*****
R429	****	*****	*****	*****	*****
R430	****	*****	*****	*****	*****
T431	****	*****	*****	*****	*****
S432	****	*****	60.98	176.01	61.99
L433	7.76	113.81	56.84	175.63	40.60
N434	6.88	114.41	51.07	178.43	40.72
L435	6.90	125.69	60.23	178.59	40.25
R436	8.29	118.42	60.50	177.70	28.25
S437	8.32	113.30	60.66	176.65	61.99
C438	7.91	119.45	64.65	175.60	25.87
I439	8.00	119.79	65.35	177.59	36.21
A440	7.67	118.17	54.14	179.15	17.37
Q441	7.16	113.64	55.27	175.31	26.94
A442	7.47	121.57	49.63	179.04	18.75
R443	7.10	119.25	59.04	174.51	28.74
N444	8.40	115.28	53.11	174.08	38.90
R445	8.03	113.38	55.83	176.86	34.12
V446	7.32	120.54	63.82	173.75	30.89
A447	8.29	125.80	50.55	175.77	20.07
F448	7.55	121.49	56.42	174.07	40.46
I449	8.34	123.61	59.59	173.22	42.79
N450	6.81	115.65	51.56	172.97	40.22
T451	****	*****	*****	*****	*****
G452	****	*****	*****	*****	
F453	****	*****	*****	*****	*****
L454	****	*****	*****	*****	*****
D455	****	*****	58.34	*****	*****
R456	7.70	116.45	56.05	179.62	*****
T457	7.62	118.04	65.59	176.54	*****
G458	7.86	111.69	47.36	174.15	
D459	8.67	120.94	57.72	181.81	43.54
E460	8.02	123.93	59.43	176.87	28.55
M461	7.67	112.65	58.66	177.16	33.18
H462	8.04	113.88	59.82	176.87	25.99
S463	****	*****	61.52	175.41	62.47
V464	7.20	111.52	58.77	172.89	28.36
M465	6.53	123.55	57.05	177.03	31.34
E466	8.72	113.90	55.70	175.93	30.39
A467	8.56	119.62	54.03	178.35	21.29
G468	6.53	101.27	42.50	178.28	
P469		*****	60.88	176.65	31.14
M470	8.91	122.28	53.24	177.15	35.07
L471	7.20	115.39	54.85	176.71	42.06
R472	8.12	116.98	58.42	176.82	29.43
K473	8.75	124.40	61.49	179.02	31.14
N474	9.45	113.97	55.18	178.72	37.08
Q475	7.47	119.28	56.78	178.48	28.13

M476	7.84	118.43	56.51	177.59	31.57
K477	7.10	114.07	58.29	175.66	31.57
S478	7.33	112.96	56.46	173.85	62.82
T479	6.78	112.10	58.72	173.72	69.19
P480		*****	64.43	180.82	30.86
W481	8.16	117.28	60.39	178.21	25.33
I482	6.01	126.80	64.16	177.49	35.97
K483	7.05	123.89	58.29	179.99	30.98
A484	7.80	122.87	53.76	178.75	19.27
Y485	8.93	123.04	59.48	177.65	37.75
E486	7.65	119.19	58.56	178.88	28.48
R487	7.40	120.73	57.80	177.78	29.20
N488	9.54	117.06	56.46	178.10	40.01
N489	7.36	121.16	57.21	175.15	40.37
V490	6.57	116.72	65.81	178.25	31.10
L491	8.52	115.98	57.48	180.28	40.13
S492	8.57	115.82	63.46	175.93	61.75
G493	8.02	109.37	47.70	174.82	
L494	8.38	122.18	57.00	171.41	39.39
F495	9.35	123.72	60.82	176.06	39.41
C496	7.38	113.13	58.99	173.26	28.01
G497	7.51	104.89	46.17	175.93	
L498	7.54	115.19	56.65	177.48	39.14
R499	8.14	120.02	58.44	177.65	29.22
G500	9.04	116.92	45.28	173.75	
K501	7.90	116.06	54.90	173.59	32.92
A502	7.54	119.42	50.06	176.26	23.06
Q503	8.20	119.33	54.58	174.81	29.93
I504	9.08	123.73	60.29	175.11	39.02
G505	8.59	110.62	44.00	175.93	
K506	7.32	119.42	54.85	178.28	34.60
G507	8.16	106.40	45.90	172.99	
M508	8.55	116.92	54.20	177.65	33.52
W509	6.86	126.66	56.37	174.62	28.50
A510	7.92	128.52	51.91	175.63	19.11
M511	5.38	116.06	53.22	175.30	31.01
P512		*****	64.38	175.09	31.10
D513	8.71	115.91	54.14	176.79	39.77
L514	7.39	126.63	53.55	177.41	38.11
M515	7.97	121.67	55.16	178.27	35.73
A516	9.89	130.38	55.06	181.81	15.59
D517	9.28	121.93	56.67	177.46	38.70
M518	7.15	122.61	58.24	179.10	29.32
Y519	9.23	120.56	60.55	178.62	37.75
S520	8.16	114.32	60.12	175.52	62.82
Q521	7.60	117.66	57.32	178.72	30.74
K522	8.63	121.16	59.42	176.68	33.84
G523	7.51	106.12	46.05	175.87	
D524	7.51	120.82	56.78	179.21	39.30
Q525	7.64	118.59	58.72	176.71	26.70
L526	6.70	117.91	56.08	180.60	39.06
R527	7.33	118.42	58.61	176.25	28.96
A528	6.98	117.57	51.28	177.03	18.08
G529	7.38	103.75	44.54	173.07	

A530	7.26	121.32	51.37	176.64	18.52
N531	8.94	113.30	50.99	174.21	38.06
T532	7.71	112.35	61.38	171.70	69.21
A533	7.52	122.09	51.42	176.23	20.19
W534	6.72	119.76	54.74	176.80	29.46
V535	8.14	113.72	56.65	176.47	33.52
P536		*****	63.85	175.09	31.82
S537	6.95	113.27	54.90	172.75	64.18
P538		*****	*****	*****	*****
T539	****	*****	66.51	175.23	67.88
A540	7.84	121.55	54.14	179.37	18.32
A541	8.27	120.82	55.43	177.49	16.30
T542	8.16	117.31	65.92	173.05	67.05
L543	7.10	114.89	55.99	178.30	40.70
H544	8.88	117.35	55.45	177.62	29.10
A545	8.18	123.13	55.39	179.58	16.24
L546	7.14	112.35	57.41	180.81	39.02
H547	7.89	117.61	59.64	178.17	29.58
Y548	7.79	119.68	58.82	176.37	35.91
H549	7.27	116.57	58.93	176.37	31.97
Q550	7.21	118.56	56.70	176.26	28.86
T551	7.73	118.04	61.24	171.00	69.21
N552	8.35	122.22	50.99	175.96	36.39
V553	8.90	124.68	64.48	177.54	30.17
Q554	7.91	119.07	58.11	179.97	26.11
S555	7.46	116.40	60.12	176.42	61.86
V556	7.92	123.47	66.19	179.31	30.29
Q557	8.23	116.06	60.02	178.00	27.18
A558	7.79	120.54	54.66	179.45	17.08
N559	8.04	117.09	55.56	178.79	37.35
I560	7.95	121.32	64.86	178.60	37.11
A561	8.02	120.11	53.44	177.05	17.20
Q562	7.31	115.45	55.37	176.45	27.90
T563	7.68	113.64	61.05	174.16	70.77
E564	8.44	123.82	54.66	177.73	26.47
F565	7.88	121.92	58.77	176.83	36.99
N566	8.27	120.37	55.34	177.32	36.75
A567	7.72	121.06	53.00	178.44	17.56
E568	7.79	115.88	57.19	177.81	29.34
F569	7.14	115.36	63.17	178.11	37.23
E570	8.52	119.90	60.45	175.79	25.33
P571		*****	65.62	179.85	29.32
L572	8.06	117.48	57.37	178.70	41.44
L573	7.92	122.61	57.75	177.97	39.77
D574	7.77	118.42	57.43	180.31	38.94
D575	7.96	123.21	57.10	179.21	40.13
L576	8.72	121.93	57.75	178.24	41.67
L577	7.48	117.40	53.87	174.37	39.89
T578	7.50	117.66	61.31	173.91	67.16
I579	7.63	123.72	58.51	176.95	36.45
P580		*****	62.68	173.94	27.65
V581	7.44	116.85	59.15	174.96	32.64
A582	8.79	128.68	50.80	176.33	18.56
E583	8.23	124.23	56.84	175.79	29.43

N584	****	*****	52.20	173.61	37.87
A585	7.94	124.75	51.18	176.84	16.42
N586	7.45	119.96	51.82	174.82	37.16
W587	6.88	119.62	58.13	176.36	28.48
S588	9.20	119.71	56.73	174.69	64.79
A589	8.89	123.72	55.06	180.63	16.78
Q590	8.34	117.14	58.72	178.27	27.30
E591	7.75	122.35	59.26	178.43	29.67
I592	8.11	119.53	64.76	177.22	37.51
Q593	7.91	118.85	57.70	177.16	27.65
Q594	8.07	117.83	58.34	178.59	27.89
E595	7.95	122.44	58.08	177.86	28.25
L596	8.24	119.11	57.91	177.32	40.37
D597	8.80	118.17	57.32	178.27	38.82
N598	7.90	116.72	56.46	178.67	38.23
N599	8.02	120.47	55.81	176.87	37.87
V600	9.22	122.01	66.73	177.65	30.77
Q601	8.95	121.14	61.05	178.74	25.21
G602	7.75	105.97	45.90	176.69	
I603	7.64	121.75	63.82	177.48	37.47
L604	8.66	118.99	57.52	178.44	43.45
G605	8.79	104.85	46.72	174.68	
Y606	7.06	118.04	60.40	179.12	38.66
V607	9.45	120.54	66.25	177.62	29.93
V608	8.46	120.37	64.91	177.48	29.22
R609	6.22	121.75	58.44	177.48	28.26
W610	7.58	125.20	62.00	178.90	31.73
V611	9.22	114.94	66.14	176.80	31.73
E612	7.54	112.61	58.33	177.48	27.66
Q613	****	*****	54.84	175.95	31.10
G614	7.12	110.39	45.81	173.53	
I615	7.38	121.58	59.96	174.07	39.30
G616	8.40	111.75	43.98	173.24	
C617	6.75	120.91	58.29	172.56	27.30
S618	9.58	125.91	58.35	171.20	62.82
K619	8.20	116.32	55.81	175.15	30.39
V620	9.05	131.92	59.15	174.74	33.35
P621		*****	61.25	177.81	30.74
D622	8.86	126.84	52.04	178.88	39.77
I623	7.50	118.08	63.68	174.82	37.99
H624	8.06	120.56	54.25	174.28	28.36
N625	8.19	114.58	54.73	173.99	36.33
V626	8.71	124.92	62.46	175.74	30.27
A627	8.64	129.25	51.91	176.09	18.04
L628	8.44	124.77	52.56	177.97	43.69
M629	9.17	127.01	54.20	173.59	33.76
E630	9.26	123.90	53.41	174.78	32.21
D631	7.18	119.25	51.21	175.63	40.94
R632	7.38	115.37	58.38	175.22	29.82
A633	7.61	123.47	54.47	179.56	19.35
T634	8.21	113.99	63.80	175.52	67.78
L635	7.80	118.57	55.30	179.92	42.06
R636	7.14	124.59	*****	*****	29.45
I637	****	*****	*****	*****	*****

S638	****	*****	*****	*****	*****
S639	****	*****	62.68	175.90	*****
Q640	7.39	119.19	57.38	176.49	28.13
H641	7.69	120.78	62.92	176.41	30.50
I642	7.35	115.95	64.33	178.48	37.51
A643	8.34	119.45	54.73	180.28	16.66
N644	8.11	119.28	57.32	176.54	39.53
W645	8.58	123.72	60.50	180.23	27.89
L646	9.00	122.70	57.48	179.82	41.91
R647	8.33	123.89	57.80	178.53	27.65
H648	7.73	115.01	56.19	174.85	30.39
G649	7.65	107.92	46.21	174.12	
I650	8.40	120.73	60.23	176.09	35.26
L651	6.72	114.26	51.16	176.30	45.95
T652	7.61	108.04	58.55	175.66	71.01
K653	9.05	123.21	60.23	178.11	30.77
E654	9.03	118.81	59.80	179.37	27.43
Q655	7.86	122.52	58.06	179.53	28.02
V656	8.04	121.75	66.41	177.16	30.17
Q657	8.89	120.71	58.77	177.65	26.95
A658	7.89	119.94	54.47	179.66	16.72
S659	7.59	114.41	61.41	177.57	62.93
L660	8.59	120.97	58.44	178.60	41.05
E661	7.72	116.14	59.26	179.20	28.26
N662	8.48	117.95	55.72	179.50	38.06
M663	9.92	119.42	55.12	179.17	33.16
A664	8.21	124.25	55.83	178.11	17.08
K665	6.99	114.94	59.15	179.31	31.25
V666	6.96	121.23	65.62	178.06	30.89
V667	8.26	122.01	65.35	179.37	30.77
D668	8.94	122.18	56.81	179.86	39.26
Q669	7.73	120.63	58.33	179.37	26.95
Q670	8.14	119.50	57.52	177.13	27.30
N671	7.15	116.83	53.16	173.75	38.42
A672	6.93	121.23	53.92	178.36	17.80
G673	8.46	107.69	44.45	173.44	
D674	7.46	122.55	50.11	176.29	40.95
P675		*****	63.62	177.06	31.10
A676	8.27	120.65	51.28	176.97	18.44
Y677	7.58	121.50	59.15	174.77	38.70
R678	7.26	129.36	51.72	172.89	29.20
P679		*****	62.06	177.14	31.10
M680	10.62	124.79	58.02	177.32	36.21
A681	9.79	121.97	52.84	178.66	16.60
G682	6.25	108.73	44.76	173.56	
N683	7.73	119.50	51.53	176.04	38.90
F684	7.11	119.76	59.09	177.40	37.11
A685	8.08	116.06	53.22	178.11	17.68
N686	7.28	112.78	51.86	174.21	39.74
S687	7.27	115.45	56.05	175.17	61.98
C688	9.48	130.54	62.63	176.31	26.83
A689	9.10	121.06	54.41	177.16	19.95
F690	7.97	119.33	61.65	177.95	38.66
K691	7.85	119.33	58.98	178.11	29.58

A692	7.43	122.01	54.63	178.47	17.56
A693	7.67	118.38	54.58	177.62	18.28
S694	7.36	109.25	61.27	175.70	62.10
D695	8.15	122.52	57.19	178.00	40.22
L696	8.27	118.64	57.16	177.70	40.46
I697	6.84	113.47	63.82	178.25	37.71
F698	8.81	117.18	61.21	178.11	36.51
L699	8.90	117.61	53.22	179.66	39.74
G700	7.35	112.48	47.97	177.81	
V701	8.79	118.21	64.89	176.26	30.41
K702	7.41	116.49	54.44	177.16	31.85
Q703	7.29	121.83	52.92	174.68	25.99
P704		*****	62.55	177.22	29.79
N705	9.48	118.64	55.06	173.43	37.51
G706	7.22	103.50	45.49	172.32	
Y707	8.14	120.82	59.58	176.17	35.49
T708	****	*****	62.08	175.39	69.67
E709	10.32	123.25	63.08	174.23	25.75
P710		*****	66.78	180.53	29.67
L711	8.42	118.51	56.78	179.04	42.03
L712	8.63	120.30	58.02	179.50	40.96
H713	9.87	117.74	60.07	177.32	27.41
A714	7.03	119.62	54.84	181.22	16.89
W715	8.23	118.25	60.39	178.56	29.20
R716	9.03	121.58	57.37	177.81	29.43
L717	8.50	121.76	58.45	179.82	40.25
R718	7.66	119.19	58.67	179.34	28.60
E719	8.44	124.66	58.99	179.99	28.13
K720	8.57	119.28	60.39	179.50	31.45
E721	7.92	118.34	57.86	178.19	28.60
S722	7.77	114.32	59.64	175.01	62.82
H723	7.70	120.16	55.80	175.09	28.75

a) The unassigned resonances are shown with asterisks (*). No attempt was made to correct carbon chemical shifts for ^2H isotope effects. The chemical shifts of ^1H and ^{15}N nuclei correspond to the TROSY component⁵ (800 MHz). ^1H and ^{13}C chemical shifts are relative to external TSP and ^{15}N shifts are relative to external ammonia.

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