JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(45), 11738-11748, DOI:10.1021/ja982019w

Supporting information for K.H. Gardner *et al.*, "Solution NMR Studies of a 42 kDa *E. coli* maltose binding protein/β-cyclodextrin complex: Chemical Shift Assignments and Analysis"

Table 1: Experimental parameters. For each dimension of every experiment, the following parameters are listed: total number of acquired points (*=complex points), [number of points in the fully processed matrix], (sweep width, maximum acquisition time). In addition, the number of scans/FID, recycle delay (R.D.) and total experimental acquisition time are listed for each experiment.

Table 2: Chemical shifts of the MBP component of the MBP/β-cyclodextrin complex. Chemical shifts listed as n/d were not determined. No attempt has been made to correct these shifts for deuterium isotope effects, which can be as large as 1 ppm (^{13}C). Assignments of the Ile Cγ2 chemical shifts were made with data from the (HM)CMC(CM)HM experiment, using the low population of Ile Cγ2 CHD_2 methyl groups present in the sample. Note that deuterium isotope effects are particularly noticeable for Ile γ2 methyl groups (e.g. compare Ile 11 and Ile 60 Cγ2 shifts in Table 2 [CHD_2] with those shown in Figure 6a [CH_3]) on account of the two deuterons directly bonded to the $^{13}C\gamma2$ methyl carbon in the deuterated, methyl-protonated sample. The assignments of Val 240 γ1 methyl group are tentative as discussed in the text, and are marked with an asterisk (*).

Table 1: Experimental parameters

BACKBONE				
	F_1 (^{13}C)	**F_2 (^{15}N)**	**F_3 (^{1}H)**	scans/R.D. total time
CT-HNCA	92* [256] (3921.6 Hz, 23.5 ms)	32* [128] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	8/1.8 s 51 hr
CT-HN(CO)CA	92* [256] (3921.6 Hz, 23.5 ms)	32* [128] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	8/2.0 s 58 hr
CT-HN(CA)CB	92* [256] (4199.9 Hz, 21.9 ms)	32* [128] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	16/2.0 s 115 hr
CT-HN(COCA)CB	92* [256] (4199.9 Hz, 21.9 ms)	32* [128] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	8/1.8 s 52 hr
HNCO	64* [256] (1621.0 Hz, 39.5 ms)	32* [64] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	8/1.2 s 25 hr
SIDECHAIN				
	F_1 (methyl ^{13}C)	**F_2 (attached ^{13}C)**	**F_3 (methyl ^{1}H)**	scans/R.D. total time
(HM)CMC(CM)HM	49* [256] (3600.0 Hz, 13.6 ms)	89* [256] (3600.0 Hz, 24.7 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	4/1.5 s 63 hr
	F_1 (methyl ^{13}C)	**F_2 (^{15}N)**	**F_3 (^{1}H)**	
(H)C(CO)NH-TOCSY	64* [256] (9178.5 Hz, 7.0 ms)	32* [64] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	32/0.8 s 71 hr
(H)C(CA)NH-TOCSY	64* [256] (8000.0 Hz, 8.0 ms)	20* [64] (1638.0 Hz, 12.2 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	32/1.0 s 63 hr
	F_1 (methyl ^{1}H)	**F_2 (^{15}N)**	**F_3 (^{1}H)**	
H(C)(CO)NH-TOCSY	64* [256] (7500.5 Hz, 8.5 ms)	32* [64] (1638.0 Hz, 19.5 ms)	576* [1024] (9000.9 Hz, 64.0 ms)	32/0.8 s 71 hr

Table 2: MBP chemical shift assignments

residue	HN	N	Cα	Cβ	CO	other
LYS 1	n/d	n/d	55.78	32.21	176.35	
THR 2	8.201	116.28	61.55	69.11	174.25	
GLU 3	8.519	122.65	55.64	30.30	175.94	
GLU 4	8.476	122.31	56.20	29.51	176.82	
GLY 5	8.574	110.38	45.22	----	172.16	
LYS 6	7.707	119.31	54.46	34.44	173.42	
LEU 7	8.385	118.69	52.84	45.57	175.17	Cγ:25.85 Cδ1:25.07 Hδ1:0.35 Cδ2:24.30 Hδ2:0.53
VAL 8	10.009	125.54	61.28	33.28	175.76	Cγ1:20.89 Hγ1:0.88 Cγ2:21.21 Hγ2:0.92
ILE 9	9.117	128.45	59.43	40.35	174.57	Cγ1:26.59 Cδ1:14.50 Hδ1:0.33 Cγ2:18.13 Hγ2:0.99
TRP 10	9.036	126.76	53.68	32.16	173.98	
ILE 11	8.701	121.99	59.35	40.71	171.01	Cγ1:27.74 Cδ1:13.15 Hδ1:0.11 Cγ2:14.23 Hγ2:0.63
ASN 12	8.854	122.59	53.87	39.21	177.26	
GLY 13	8.224	106.53	45.88	----	173.10	
ASP 14	7.923	116.76	52.58	39.14	176.03	
LYS 15	7.558	118.65	52.50	32.32	177.35	
GLY 16	8.732	107.96	47.56	----	175.56	
TYR 17	8.203	120.51	59.21	37.03	177.02	
ASN 18	8.095	123.44	55.68	36.88	178.89	
GLY 19	8.929	111.60	46.94	----	175.82	
LEU 20	8.302	121.78	57.09	40.70	178.61	Cγ:26.32 Cδ1:24.78 Hδ1:0.87 Cδ2:26.81 Hδ2:0.64
ALA 21	8.074	121.08	54.59	16.80	180.49	
GLU 22	7.792	120.44	59.19	27.95	180.03	
VAL 23	7.811	123.02	66.26	30.96	179.34	Cγ1:22.31 Hγ1:0.82 Cγ2:23.49 Hγ2:1.26
GLY 24	8.696	106.72	47.11	----	175.02	
LYS 25	8.278	122.71	58.75	31.13	179.38	
LYS 26	7.638	122.72	59.16	31.31	178.02	
PHE 27	8.061	120.10	60.87	38.59	178.86	
GLU 28	8.892	124.14	58.56	29.13	179.75	
LYS 29	8.081	121.90	58.76	30.68	178.22	
ASP 30	7.559	116.37	55.97	40.36	178.16	
THR 31	7.908	107.20	62.22	71.63	176.10	
GLY 32	8.587	112.69	44.87	----	173.35	
ILE 33	7.739	124.22	58.25	35.13	173.62	Cγ1:25.05 Cδ1:10.25 Hδ1:0.58 Cγ2:16.03 Hγ2:0.63
LYS 34	7.701	124.60	56.00	32.14	175.52	
VAL 35	8.461	124.77	60.57	32.67	175.61	Cγ1:20.78 Hγ1:0.36 Cγ2:22.48 Hγ2:0.78
THR 36	9.115	125.13	60.89	70.36	172.50	
VAL 37	8.859	127.36	60.98	31.98	175.17	Cγ1:22.85 Hγ1:0.96 Cγ2:20.67 Cγ2:0.77
GLU 38	9.613	126.96	53.74	32.50	173.34	
HIS 39	8.300	115.27	50.80	27.99	n/d	
PRO 40	----	n/d	61.73	30.09	176.58	
ASP 41	8.203	121.15	54.30	40.45	176.30	
LYS 42	8.752	119.32	55.95	28.78	178.27	
LEU 43	7.413	120.01	58.96	40.18	175.79	Cγ:25.80 Cδ1:26.61 Hδ1:1.10 Cδ2:26.52 Hδ2:1.12
GLU 44	10.393	123.80	56.54	24.11	178.38	
GLU 45	7.330	120.66	56.03	29.39	178.10	
LYS 46	8.205	120.21	57.91	32.71	178.94	
PHE 47	8.569	117.14	62.86	35.53	n/d	
PRO 48	----	n/d	64.95	29.50	177.67	

GLN 49	6.940	114.64	57.37	27.97	178.19	
VAL 50	7.569	110.18	61.30	31.99	177.96	Cγ1:21.12 Hγ1:0.97 Cγ2:19.73 Hγ2:0.86
ALA 51	8.075	124.92	54.46	17.16	179.71	
ALA 52	7.706	117.58	52.61	17.58	178.32	
THR 53	7.251	106.34	61.03	69.44	175.14	
GLY 54	7.843	109.03	45.02	----	173.40	
ASP 55	7.555	119.25	52.94	41.65	175.08	
GLY 56	8.149	106.42	43.51	----	n/d	
PRO 57	----	n/d	61.26	30.03	174.83	
ASP 58	8.711	117.91	57.69	43.12	175.44	
ILE 59	7.621	114.48	58.40	42.00	173.54	Cγ1:26.61 Cδ1:13.81 Hδ1:0.74 Cγ2:18.25 Hγ2:0.81
ILE 60	8.880	124.33	57.44	40.76	172.72	Cγ1:28.12 Cδ1:14.63 Hδ1:0.41 Cγ2:13.33 Hγ2:0.04
PHE 61	8.630	126.04	55.20	41.46	176.47	
TRP 62	9.168	121.30	56.79	31.09	173.45	
ALA 63	6.387	126.17	53.30	18.12	179.53	
HIS 64	8.096	116.19	59.70	29.57	178.18	
ASP 65	7.714	119.24	56.08	38.48	177.57	
ARG 66	7.008	117.09	54.30	29.25	177.28	
PHE 67	7.641	116.54	57.59	35.92	177.75	
GLY 68	7.341	107.42	47.03	----	175.63	
GLY 69	7.737	107.60	46.36	----	178.03	
TYR 70	6.885	119.06	56.50	35.18	178.20	
ALA 71	8.586	122.77	53.75	17.31	181.90	
GLN 72	8.623	122.51	57.99	27.01	177.56	
SER 73	7.318	112.02	58.53	63.46	173.53	
GLY 74	8.036	109.33	45.81	----	175.95	
LEU 75	7.829	113.77	55.05	41.97	177.48	Cγ:25.58 Cδ1:25.73 Hδ1:0.64 Cδ2:20.69 Hδ2:0.52
LEU 76	7.426	116.04	52.03	42.90	176.49	Cγ:26.53 Cδ1:27.20 Hδ1:0.86 Cδ2:21.77 Hδ2:0.52
ALA 77	9.024	125.98	50.45	18.31	176.22	
GLU 78	8.186	120.91	55.76	28.77	176.55	
ILE 79	8.174	122.77	59.10	38.45	175.46	Cγ1:25.50 Cδ1:12.33 Hδ1:0.17 Cγ2:17.58 Hγ2:0.65
THR 80	8.734	112.71	57.26	68.68	n/d	
PRO 81	----	n/d	64.12	31.10	177.05	
ASP 82	7.483	112.70	49.07	39.38	n/d	
LYS 83	n/d	n/d	59.22	31.08	177.47	
ALA 84	8.193	119.41	54.22	16.90	180.13	
PHE 85	7.917	118.53	61.72	38.48	178.10	
GLN 86	8.491	117.15	59.12	27.66	179.85	
ASP 87	8.064	116.88	55.52	40.29	176.31	
LYS 88	7.791	117.17	57.58	31.33	176.58	
LEU 89	7.650	120.03	52.91	41.98	176.53	Cγ:28.10 Cδ1:26.11 Hδ1:0.55 Cδ2:25.23 Hδ2:0.50
TYR 90	7.717	117.01	58.47	38.39	n/d	
PRO 91	----	n/d	66.22	30.83	179.35	
PHE 92	8.008	112.69	58.70	36.12	176.16	
THR 93	7.103	111.04	64.14	66.51	176.22	
TRP 94	6.663	119.82	57.96	28.79	178.10	
ASP 95	7.254	115.51	56.67	39.33	178.22	
ALA 96	6.996	118.60	53.10	17.17	176.66	
VAL 97	6.974	106.05	59.14	30.27	172.46	Cγ1:22.21 Hγ1:0.59 Cγ2:19.48 Hγ2:1.35
ARG 98	7.037	121.27	54.28	30.95	176.40	
TYR 99	9.686	126.76	57.76	41.23	n/d	

ASN 100	n/d	n/d	53.26	36.54	175.13	
GLY 101	8.591	102.20	44.97	----	173.75	
LYS 102	7.759	121.18	54.02	34.07	175.04	
LEU 103	8.948	123.36	54.59	41.61	178.27	Cγ:25.97 Cδ1:24.82 Hδ1:0.52 Cδ2:24.24 Hδ2:0.99
ILE 104	8.806	112.70	59.11	38.51	175.30	Cγ1:26.68 Cδ1:14.65 Hδ1:0.86 Cγ2:19.64 Hγ2:0.87
ALA 105	7.669	117.21	51.48	21.39	173.51	
TYR 106	8.958	113.72	55.40	39.35	n/d	
PRO 107	----	n/d	61.76	32.19	174.36	
ILE 108	8.500	115.41	60.33	37.08	176.34	Cγ1:25.27 Cδ1:10.05 Hδ1:0.65 Cγ2:15.89 Hγ2:0.84
ALA 109	7.872	118.31	50.08	22.60	174.48	
VAL 110	8.759	120.94	61.36	33.86	173.52	Cγ1: 21.17 Hγ1:0.75 Cγ2:20.75 Hγ2:0.51
GLU 111	9.559	123.49	54.37	32.51	173.65	
ALA 112	6.379	117.45	50.28	21.47	176.30	
LEU 113	8.420	122.97	54.54	42.78	173.34	Cγ:25.06 Cδ1:26.85 Hδ1:0.72 Cδ2:23.63 Hδ2:0.85
SER 114	7.464	107.98	56.55	66.69	171.74	
LEU 115	7.280	122.09	53.81	43.07	173.98	Cγ:26.63 Cδ1:22.83 Hδ1:0.68 Cδ2:24.61 Hδ2:0.59
ILE 116	8.642	129.56	59.47	37.55	174.37	Cγ1:26.38 Cδ1:13.72 Hδ1:0.46 Cγ2:17.31 Hγ2:0.45
TYR 117	9.057	121.73	54.00	41.62	172.68	
ASN 118	9.302	121.14	51.56	37.12	175.51	
LYS 119	8.786	125.46	58.11	31.95	177.42	
ASP 120	8.146	115.60	55.77	39.81	177.38	
LEU 121	7.112	117.77	54.84	43.42	176.47	Cγ:26.07 Cδ1:24.73 Hδ1:0.67 Cδ2:22.79 Hδ2:0.78
LEU 122	8.319	119.84	51.13	43.41	n/d	Cγ:26.05 Cδ1:25.62 Hδ1:0.94 Cδ2:26.78 Hδ2:0.95
PRO 123	----	n/d	61.79	31.03	177.32	
ASN 124	9.062	123.61	52.96	40.94	n/d	
PRO 125	----	n/d	n/d	n/d	n/d	
PRO 126	----	n/d	61.77	30.57	175.84	
LYS 127	8.117	118.47	55.97	32.56	177.15	
THR 128	7.863	108.68	59.46	71.23	174.34	
TRP 129	10.152	123.81	60.39	27.94	179.65	
GLU 130	10.571	117.99	61.15	27.55	178.37	
GLU 131	7.595	116.64	56.55	30.63	176.73	
ILE 132	8.186	121.55	66.32	33.44	n/d	Cγ1:29.58 Cδ1:12.40 Hδ1:0.56 Cγ2:16.11 Hγ2:0.79
PRO 133	----	n/d	66.48	29.86	177.45	
ALA 134	7.803	118.07	54.61	17.29	180.99	
LEU 135	7.602	120.01	56.81	41.35	179.00	Cγ:26.23 Cδ1:24.03 Hδ1:0.89 Cδ2:24.24 Hδ2:0.89
ASP 136	8.817	118.53	58.41	41.26	177.12	
LYS 137	8.029	117.27	59.76	31.39	179.58	
GLU 138	7.467	118.55	58.62	28.79	179.50	
LEU 139	8.396	121.20	57.38	39.74	180.40	Cγ:27.24 Cδ1:25.91 Hδ1:0.79 Cδ2:23.01 Hδ2:0.85
LYS 140	9.247	124.09	58.28	31.26	181.33	
ALA 141	7.255	121.99	53.81	17.17	178.37	
LYS 142	7.636	115.77	54.42	31.73	176.49	
GLY 143	7.870	107.74	45.52	----	174.07	
LYS 144	7.849	119.88	52.74	34.52	173.57	
SER 145	7.567	109.46	56.05	65.83	174.42	
ALA 146	9.573	122.81	55.07	17.33	175.66	
LEU 147	8.663	116.82	53.82	44.88	174.82	Cγ:27.42 Cδ1:22.49 Hδ1:0.69 Cδ2:27.60 Hδ2:0.94
MET 148	8.177	121.57	55.22	37.20	174.05	
PHE 149	8.566	120.07	55.15	40.83	171.33	
ASN 150	8.651	115.86	52.76	36.64	172.35	

LEU 151	7.303	123.03	53.86	41.26	177.74	Cγ:25.78 Cδ1:26.24 Hδ1:0.75 Cδ2:23.62 Hδ2:0.15
GLN 152	7.930	113.02	55.00	27.79	175.84	
GLU 153	6.448	113.71	50.81	32.46	n/d	
PRO 154	----	n/d	63.04	31.46	176.66	
TYR 155	7.929	117.70	61.91	39.54	175.60	
PHE 156	8.048	112.05	60.03	40.95	175.85	
THR 157	7.577	105.90	62.35	68.67	175.75	
TRP 158	8.353	124.11	60.12	28.02	n/d	
PRO 159	----	n/d	65.26	29.43	177.85	
LEU 160	6.410	111.47	55.37	41.55	176.52	Cγ:25.60 Cδ1:19.56 Hδ1:-1.01 Cδ2:25.12 Hδ2:-0.29
ILE 161	6.953	119.39	65.03	36.78	175.37	Cγ1:27.91 Cδ1:13.14 Hδ1:0.76 Cγ2:16.04 Hγ2:0.48
ALA 162	7.977	115.12	51.65	17.76	179.35	
ALA 163	6.644	120.71	55.72	19.06	178.01	
ASP 164	9.555	114.91	52.78	41.76	176.38	
GLY 165	7.471	103.61	45.14	----	175.44	
GLY 166	7.388	108.04	44.79	----	171.92	
TYR 167	8.255	115.47	56.99	38.50	173.15	
ALA 168	10.481	124.25	52.58	15.89	172.88	
PHE 169	6.304	107.99	55.03	42.02	176.46	
LYS 170	8.856	125.55	56.45	31.81	174.46	
TYR 171	8.582	129.74	55.71	39.21	174.64	
GLU 172	8.223	126.72	55.13	31.89	n/d	
ASN 173	n/d	n/d	53.53	36.68	175.18	
GLY 174	7.452	101.99	45.07	----	172.98	
LYS 175	7.072	118.52	53.96	34.71	174.47	
TYR 176	8.709	119.87	58.28	39.22	176.01	
ASP 177	9.002	123.83	52.27	40.68	177.22	
ILE 178	7.707	116.93	62.97	36.22	175.58	Cγ1:24.93 Cδ1:13.92 Hδ1:0.86 Cγ2:17.53 Hγ2:0.62
LYS 179	8.284	116.06	54.12	31.35	176.25	
ASP 180	7.752	123.22	52.73	40.33	172.79	
VAL 181	7.463	122.79	58.71	34.49	176.64	Cγ1:21.59 Hγ1:0.82 Cγ2:22.59 Hγ2:0.71
GLY 182	7.059	120.68	45.82	----	173.95	
VAL 183	6.697	113.96	62.76	32.32	173.02	Cγ1:22.42 Hγ1:0.88 Cγ2:22.41 Hγ2:0.84
ASP 184	7.831	114.79	51.01	39.20	175.99	
ASN 185	6.887	116.23	51.03	38.77	n/d	
ALA 186	n/d	n/d	54.88	17.59	180.23	
GLY 187	8.360	109.35	46.71	----	175.76	
ALA 188	8.053	127.62	53.31	17.70	180.55	
LYS 189	7.975	115.17	59.05	31.24	180.07	
ALA 190	8.206	124.63	55.11	17.23	181.05	
GLY 191	8.210	107.51	47.26	----	174.76	
LEU 192	8.652	121.16	56.63	39.53	178.14	Cγ:26.30 Cδ1:24.25 Hδ1:1.09 Cδ2:25.29 Hδ2:0.85
THR 193	8.527	116.39	67.44	68.01	174.97	
PHE 194	7.645	122.01	61.72	38.54	177.20	
LEU 195	7.714	119.50	58.05	40.65	177.88	Cγ:26.49 Cδ1:23.70 Hδ1:0.90 Cδ2:25.22 Hδ2:0.85
VAL 196	8.583	117.48	66.66	30.54	178.20	Cg1:21.65 Hγ1:0.97 Cγ2:23.40 Hγ2:0.86
ASP 197	8.573	122.89	57.40	39.28	179.11	
LEU 198	7.876	120.15	57.90	41.44	178.86	Cγ:25.39 Cδ1:25.60 Hδ1:1.02 Cδ2:23.40 Hδ2:0.81
ILE 199	7.435	119.95	62.69	37.66	180.84	Cγ1:27.97 Cδ1:14.23 Hδ1:0.75 Cγ2:17.04 Hγ2:0.99
LYS 200	9.382	124.44	59.28	31.49	178.55	
ASN 201	7.988	113.88	52.99	38.06	172.98	

LYS 202	7.923	111.41	56.92	26.70	175.54	
HIS 203	8.346	116.20	56.62	27.91	175.36	
MET 204	7.463	114.06	54.03	36.77	172.96	
ASN 205	8.692	118.55	51.54	39.63	175.91	
ALA 206	9.059	124.94	54.05	17.64	176.13	
ASP 207	8.160	112.76	53.11	39.28	176.26	
THR 208	7.320	116.46	66.10	68.44	173.03	
ASP 209	6.978	130.73	51.24	41.49	175.59	
TYR 210	7.843	117.36	62.75	38.46	178.15	
SER 211	8.191	114.62	61.24	62.20	177.30	
ILE 212	8.967	124.42	64.32	37.98	178.69	Cγ1:28.10 Cδ1:13.10 Hδ1:0.87 Cγ2:16.85 Hγ2:0.95
ALA 213	7.607	120.63	54.79	16.43	177.63	
GLU 214	7.860	117.33	58.35	29.26	n/d	
ALA 215	n/d	n/d	n/d	n/d	n/d	
ALA 216	n/d	n/d	54.39	19.13	180.43	
PHE 217	8.321	119.38	62.24	37.49	n/d	
ASN 218	n/d	n/d	54.91	n/d	176.51	
LYS 219	7.706	116.69	55.49	32.22	177.49	
GLY 220	7.709	108.65	45.51	----	174.92	
GLU 221	8.353	116.37	56.79	29.82	175.56	
THR 222	6.845	110.49	57.44	69.90	172.51	
ALA 223	8.667	127.27	54.02	19.78	176.21	
MET 224	8.065	114.24	54.00	39.52	173.71	
THR 225	9.137	113.25	58.97	70.32	171.15	
ILE 226	7.143	122.55	59.71	39.81	174.50	Cγ1:26.88 Cδ1:11.81 Hδ1:0.07 Cγ2:17.57 Hγ2:0.85
ASN 227	8.417	121.73	51.83	42.19	175.29	
GLY 228	8.241	110.65	41.78	----	n/d	
PRO 229	----	n/d	n/d	n/d	n/d	
TRP 230	n/d	n/d	n/d	n/d	n/d	
ALA 231	n/d	n/d	n/d	n/d	n/d	
TRP 232	n/d	n/d	n/d	n/d	n/d	
SER 233	n/d	n/d	n/d	n/d	n/d	
ASN 234	n/d	n/d	n/d	n/d	n/d	
ILE 235	n/d	n/d	n/d	n/d	n/d	
ASP 236	n/d	n/d	n/d	n/d	n/d	
THR 237	n/d	n/d	n/d	n/d	n/d	
SER 238	n/d	n/d	n/d	n/d	n/d	
LYS 239	n/d	n/d	62.10	29.14	176.06	
VAL 240	5.970	111.92	58.52	25.91	176.18	Cγ1*:20.92 Hγ1*:0.59
ASN 241	6.964	125.24	51.50	n/d	173.17	
TYR 242	7.861	121.68	54.15	40.93	174.19	
GLY 243	8.498	107.40	42.39	----	170.92	
VAL 244	8.213	120.69	60.89	34.01	174.61	Cγ1:22.00 Hγ1:1.07 Cγ2:21.55 Hγ2:0.62
THR 245	9.475	119.53	58.38	70.89	173.97	
VAL 246	8.128	123.40	61.76	31.90	174.86	Cγ1:20.50 Hγ1:0.98 Cγ2:21.60 Hγ2:0.98
LEU 247	8.573	125.41	53.81	39.74	n/d	Cγ:27.70 Cδ1:25.83 Hδ1:0.66 Cδ2:23.89 Hδ2:0.65
PRO 248	----	n/d	61.35	29.69	175.32	
THR 249	8.785	111.59	60.37	70.73	174.34	
PHE 250	9.556	121.84	56.20	41.16	174.42	
LYS 251	10.552	129.60	56.73	27.63	177.44	
GLY 252	9.010	103.50	44.46	----	173.65	

GLN 253	8.227	122.29	51.73	28.74	n/d	
PRO 254	----	n/d	62.66	30.60	178.35	
SER 255	7.971	117.90	61.51	64.26	173.32	
LYS 256	7.646	123.30	52.45	32.69	n/d	
PRO 257	----	n/d	61.65	30.83	176.91	
PHE 258	9.326	118.38	57.84	39.47	177.39	
VAL 259	8.747	121.83	61.34	33.56	176.25	Cγ1:21.69 Hγ1:0.93 Cγ2:22.73 Hγ2:1.01
GLY 260	8.845	115.96	44.25	----	171.35	
VAL 261	11.034	129.08	59.61	32.51	179.12	Cγ1:20.33 Hγ1:0.70 Cγ2:21.10 Hγ2:0.56
LEU 262	8.807	134.21	55.98	40.39	174.97	Cγ:26.97 Cδ1:22.68 Hδ1:0.81 Cδ2:25.25 Hδ2:0.89
SER 263	8.765	126.56	58.17	65.54	170.46	
ALA 264	9.127	123.64	49.24	20.24	175.94	
GLY 265	9.411	110.68	42.32	----	170.87	
ILE 266	10.279	123.63	59.20	38.98	175.00	Cγ1:27.14 Cδ1:13.82 Hδ1:0.93 Cγ2:15.82 Hγ2:0.81
ASN 267	8.178	125.61	52.88	38.18	177.02	
ALA 268	8.832	130.97	54.67	17.26	178.18	
ALA 269	8.165	118.14	50.74	17.93	177.85	
SER 270	7.530	113.58	55.53	63.83	n/d	
PRO 271	----	n/d	62.99	30.57	175.76	
ASN 272	8.772	119.51	52.04	39.88	176.03	
LYS 273	7.816	119.21	61.06	31.14	178.61	
GLU 274	8.805	118.21	59.32	27.42	179.49	
LEU 275	7.445	120.70	56.74	41.54	178.18	Cγ:26.24 Cδ1:25.42 Hδ1:0.95 Cδ2:22.70 Hδ2:0.96
ALA 276	8.309	120.31	54.79	17.21	178.33	
LYS 277	7.812	118.22	59.60	31.77	177.01	
GLU 278	7.597	118.79	59.04	28.61	179.01	
PHE 279	8.396	118.37	61.03	37.81	177.32	
LEU 280	8.343	119.93	57.67	40.13	176.88	Cγ:26.93 Cδ1:25.78 Hδ1:0.67 Cδ2:23.43 Hδ2:0.72
GLU 281	8.405	112.88	58.92	28.86	176.82	
ASN 282	7.730	108.87	52.47	38.45	174.99	
TYR 283	7.162	116.28	59.18	37.35	176.02	
LEU 284	8.070	121.29	57.55	40.45	176.70	Cγ:26.90 Cδ1:23.92 Hδ1:0.85 Cδ2:27.32 Hδ2:1.05
LEU 285	7.817	119.22	53.83	37.82	174.72	Cγ:27.47 Cδ1:25.70 Hδ1:1.06 Cδ2:24.05 Hδ2:1.12
THR 286	8.533	108.71	58.31	72.92	174.05	
ASP 287	8.505	122.01	57.79	38.99	177.53	
GLU 288	8.404	115.59	58.67	28.59	179.86	
GLY 289	8.314	112.87	46.31	----	175.01	
LEU 290	8.190	119.45	56.68	41.00	178.64	Cγ:25.33 Cδ1:27.90 Hδ1:1.08 Cδ2:21.85 Hδ2:0.80
GLU 291	7.725	120.91	58.82	28.46	177.93	
ALA 292	7.176	119.81	54.65	17.00	180.53	
VAL 293	7.249	115.82	66.70	31.51	176.79	Cγ1:21.42 Hγ1:1.00 Cγ2:22.25 Hγ2:0.90
ASN 294	8.689	117.36	55.62	40.35	176.12	
LYS 295	8.246	115.97	57.79	31.48	177.16	
ASP 296	7.272	118.79	55.53	41.47	175.89	
LYS 297	7.625	115.85	52.01	34.11	n/d	
PRO 298	----	n/d	62.58	31.04	178.56	
LEU 299	8.598	122.43	55.06	43.18	177.24	Cγ:26.48 Cδ1:26.68 Hδ1:0.91 Cδ2:22.96 Hδ2:0.81
GLY 300	8.122	104.05	43.76	----	173.60	
ALA 301	7.507	123.83	50.85	18.78	177.42	
VAL 302	8.155	110.31	59.06	35.02	173.42	Cγ1:22.33 Hγ1:1.07 Cγ2:19.00 Hγ2:1.26
ALA 303	7.632	117.09	52.48	18.83	175.51	

LEU 304	6.376	114.99	53.71	43.41	175.24	Cγ:26.35 Cδ1:24.32 Hδ1:0.85 Cδ2:26.52 Hδ2:0.71
LYS 305	8.039	129.38	59.90	31.12	178.38	
SER 306	8.724	112.26	60.77	59.90	176.84	
TYR 307	6.631	122.21	58.50	37.97	177.16	
GLU 308	8.489	121.34	57.38	25.26	177.52	
GLU 309	7.731	115.49	58.62	28.38	178.56	
GLU 310	6.873	117.49	57.25	28.59	178.99	
LEU 311	8.220	120.95	56.54	41.20	179.37	Cγ:25.12 Cδ1:26.26 Hδ1:0.89 Cδ2:22.65 Hδ2:0.80
ALA 312	8.553	117.95	53.39	16.43	176.43	
LYS 313	7.093	117.33	58.22	31.22	177.86	
ASP 314	8.286	121.20	49.99	40.79	n/d	
PRO 315	----	n/d	63.86	31.50	178.91	
ARG 316	8.437	116.86	57.84	28.78	179.57	
ILE 317	7.525	122.90	63.91	35.81	177.72	Cγ1:28.86 Cδ1:12.54 Hδ1:1.11 Cγ2:17.18 Hγ2:0.93
ALA 318	7.852	122.56	55.21	16.68	181.04	
ALA 319	8.128	118.67	54.58	17.32	178.61	
THR 320	7.335	114.75	67.44	68.25	175.14	
MET 321	8.149	119.30	56.47	30.78	177.12	
GLU 322	8.227	121.37	59.28	28.25	179.19	
ASN 323	8.282	115.22	56.30	38.60	176.78	
ALA 324	8.085	119.66	53.81	17.06	179.96	
GLN 325	8.239	116.20	57.73	27.39	177.51	
LYS 326	7.049	117.72	55.52	32.08	175.91	
GLY 327	7.243	106.36	44.03	----	172.33	
GLU 328	8.516	121.71	53.34	32.24	176.47	
ILE 329	9.159	127.88	61.68	37.14	177.93	Cγ1:26.86 Cδ1:12.34 Hδ1:0.82 Cγ2:16.75 Hγ2:0.81
MET 330	8.478	124.94	55.90	33.77	n/d	
PRO 331	----	n/d	62.96	30.58	175.16	
ASN 332	7.588	118.14	50.93	37.80	175.37	
ILE 333	6.371	108.50	58.96	36.03	n/d	Cγ1:24.62 Cδ1:12.28 Hδ1:-0.15 Cγ2:19.04 Hγ2:1.15
PRO 334	----	n/d	64.81	30.71	178.49	
GLN 335	8.346	116.46	58.79	25.84	176.80	
MET 336	7.832	118.37	55.43	29.68	n/d	
SER 337	n/d	n/d	n/d	n/d	176.97	
ALA 338	7.345	122.93	54.02	17.97	179.74	
PHE 339	7.514	118.84	61.16	38.33	176.32	
TRP 340	8.769	118.02	59.38	29.72	178.77	
TYR 341	7.426	114.62	60.79	37.80	178.35	
ALA 342	8.420	121.85	54.28	18.48	180.59	
VAL 343	8.658	118.42	66.38	30.46	176.83	Cγ1:21.26 Hγ1:0.86 Cγ2:23.25 Hγ2:0.14
ARG 344	8.105	120.78	59.66	29.31	178.22	
THR 345	7.524	113.59	65.85	68.62	174.84	
ALA 346	7.785	122.84	54.85	18.05	178.93	
VAL 347	8.139	115.90	66.91	30.84	177.75	Cγ1:20.52 Hγ1:0.93 Cγ2:22.34 Hγ2:1.05
ILE 348	7.759	118.32	64.28	36.80	180.02	Cγ1:28.63 Cδ1:13.07 Hδ1:0.87 Cγ2:16.24 Hγ2:0.91
ASN 349	8.807	121.04	55.25	36.54	177.77	
ALA 350	8.500	122.69	53.37	17.29	180.86	
ALA 351	9.141	120.99	54.93	17.33	178.03	
SER 352	7.875	107.89	58.28	63.75	175.45	
GLY 353	7.606	109.76	45.13	----	174.29	
ARG 354	8.212	121.01	57.84	30.12	176.56	

GLN 355	7.322	113.57	53.62	35.71	175.82	
THR 356	8.550	111.70	60.77	69.90	174.69	
VAL 357	8.710	121.30	67.29	31.00	176.89	Cγ1:21.32 Hγ1:0.99 Cγ2:23.41 Hγ2:1.05
ASP 358	8.101	115.12	57.03	40.29	178.65	
GLU 359	7.587	118.60	58.19	29.51	178.34	
ALA 360	8.681	121.46	54.21	17.67	181.26	
LEU 361	8.059	116.15	56.83	39.19	178.65	Cγ:26.01 Cδ1:25.23 Hδ1:0.90 Cδ2:19.59 Hδ2:0.72
LYS 362	7.680	121.48	59.14	30.89	179.63	
ASP 363	8.132	120.03	56.64	39.82	178.64	
ALA 364	7.727	121.23	54.66	17.13	178.15	
GLN 365	8.230	118.12	59.73	26.72	179.01	
THR 366	8.143	115.20	65.51	68.35	175.70	
ARG 367	7.951	120.04	58.23	29.20	178.45	
ILE 368	7.986	117.30	64.27	38.07	176.91	Cγ1:28.35 Cδ1:15.28 Hδ1:0.68 Cγ2:19.30 Hγ2:1.02
THR 369	7.629	107.07	61.88	69.75	174.05	
LYS 370	7.390	128.20	58.27	31.89	n/d	