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Supplementary material

Solution Structure of Oxidised Rat Microsomal Cytochrome *b*₅

- ¹H Chemical Shifts
- Experimental NOE intensities
- Stereospecific Assignment

Chemical shifts (ppm) of oxidised rat microsomal cytochrome b₅ (A form). Data were obtained using a 800 MHz Bruker avance spectrometer, on a approximately 4mM protein sample in 1mM phosphate buffer at pH 7.0, at 298K.

Residue		HN	H α	H β	others
Asp	1				
Lys	2	8.04	4.18	1.76	H γ 1.35; H δ 1.66; H ϵ 2.96
Asp	3	8.11	4.45	2.55, 2.45	
Val	4	7.66	3.67	1.51	γ CH ₃ 0.58, 0.24
Lys	5	8.04	4.00	1.51	H γ 1.08, 0.95; H δ 1.57; H ϵ 2.84, 2.70
Tyr	6	8.10	5.57	2.52, 2.74	H δ 6.76; H ϵ 6.51
Tyr	7	8.57	5.05	3.04, 2.32	H δ 6.78; H ϵ 6.44
Thr	8	9.08	4.48	4.76	γ CH ₃ 1.12
Leu	9	9.64	3.89	1.59, 1.39	H γ 1.56; δ CH ₃ 0.93, 0.80
Glu	10	8.32	3.81	2.08, 1.83	H γ 2.19, 2.06
Glu	11	7.59	3.95	2.33, 2.19	H γ 2.63
Ile	12	8.34	3.52	1.77	H γ 1.94, 0.63; γ CH ₃ 0.88
Gln	13	8.01	4.12	2.04, 1.93	H γ 2.46
Lys	14	7.21	3.95	1.28	H γ 1.17; H δ 1.50; H ϵ 2.79
His	15	7.54	4.03	2.24, 1.49	H δ 2 6.69; H ϵ 1 7.84
Lys	16	7.44	4.69	1.29	H γ 1.11; H δ 1.60; H ϵ 2.95
Asp	17	8.01	4.88	3.06, 2.67	
Ser	18				
Lys	19	8.04	4.24	1.82	H γ 1.41; H δ 1.63 ;H ϵ 2.96
Ser	20	7.42	4.95	3.81, 3.70	
Thr	21	8.61	4.37	3.58	γ CH ₃ 0.77
Trp	22	8.53	6.06	2.88, 2.63	H δ 1 6.74; H ϵ 3 6.48; H ϵ 1 8.71; H ζ 2 6.56; H ζ 3 5.69; H η 6.29
Val	23	8.26	4.36	1.01	γ CH ₃ -0.30, -0.58
Ile	24	7.80	4.85	1.28	H γ 0.56, 0.42
Leu	25	8.47	4.32	1.11, 0.04	H γ -0.22; δ CH ₃ -2.28, -0.96
His	26	9.28	3.79	3.10	H δ 2 7.07; H ϵ 1 8.50
His	27	8.61	3.75	3.58, 3.17	H δ 2 6.85; H ϵ 1 7.82
Lys	28	8.15	4.67	1.99	H γ 1.51; H δ 1.86; H ϵ 2.96
Val	29	8.23	3.96	0.92	γ CH ₃ -0.08, 0.47
Tyr	30	8.67	4.35	1.90, 1.59	H δ 6.36; H ϵ 6.32
Asp	31	8.00	4.84	2.83, 2.56	
Leu	32	8.40	4.15	1.50	H γ 0.80; δ CH ₃ -0.93, -0.32
Thr	33	8.64	3.66	4.28	γ CH ₃ 1.35
Lys	34	9.13	4.54	2.22, 1.95	H γ 1.66, 1.60; H δ 1.82; H ϵ 3.10
Phe	35	8.08	5.12	2.74, 2.55	H δ 7.40; H ϵ 8.32; H ζ 7.62
Leu	36	7.78	4.82	2.46, 2.36	H γ 2.06; δ CH ₃ 1.24, 1.18
Glu	37	8.61	4.90	2.50, 2.35	H γ 2.65
Glu	38	8.34	4.88	2.50, 2.43	H γ 2.62, 2.56
His	39	9.01	6.96	16.61, 7.42	H δ 1 12.64
Pro	40		4.10	0.66, -3.41	H γ 1.30, -0.44
Gly	41		4.41		

Gly	42	10.54	6.06, 5.78		
Glu	43	9.99	5.88	2.89, 2.78	
Glu	44	9.56	4.24	2.49, 2.33	H γ 2.61
Val	45	9.44	4.08	2.31	γ CH ₃ 1.66, 1.54
Leu	46	7.37	3.05	2.73, 2.59	H γ 2.44; δ CH ₃ 0.72, 0.54
Arg	47	8.33	3.79	1.93	H γ 1.69, H δ 3.30
Glu	48	8.12	3.91	1.95, 1.85	H γ 2.37, 2.21
Gln	49	6.62	4.04	1.69, 0.77	H γ 1.97, 1.85
Ala	50	6.81	3.78	1.44	
Gly	51	9.26	3.72, 3.46		
Gly	52	7.27	4.06, 3.50		
Asp	53	8.32	4.52	2.64	
Ala	54	8.26	4.65	-0.04	
Thr	55	7.80	2.84	3.81	γ CH ₃ 0.37
Glu	56	8.55	3.92	2.25, 1.18	
Asn	57	7.71	4.30	2.15, 1.73	
Phe	58	8.02		2.91	
Glu	59	8.92	5.60	2.80, 2.44	H γ 3.17, 3.05
Asp	60	9.12	4.84	3.04, 2.86	
Val	61	8.25	4.45	2.54	γ CH ₃ 1.53
Gly	62	8.99	5.13, 4.85		
His	63	11.11	7.51	10.35, 9.94	H ϵ 1 $\approx$ -14.1
Ser	64	11.76	4.96	4.51, 4.21	
Thr	65	9.35	4.75	1.55	
Asp	66	8.36	4.46	2.57, 2.47	
Ala	67	8.88	4.10	0.99	
Arg	68	9.28	4.59	2.91, 2.61	H γ 2.57, H δ 3.18
Glu	69	8.96	4.23	2.17	H γ 2.39, 2.27
Leu	70	8.35	4.16	1.95, 1.72	H γ 1.44; δ CH ₃ 0.99, 0.95
Ser	71	8.30	3.65	3.27	
Lys	72	7.17	3.94	1.86, 1.71	
Thr	73	7.63	3.77	3.64	γ CH ₃ 0.77
Tyr	74	7.29	4.41	2.19, 3.32	H δ 6.81; H ϵ 6.28
Ile	75	6.68	3.25	1.30	H γ 1.17, 0.62; γ CH ₃ 0.72; δ CH ₃ 0.34
Ile	76	8.57	4.48	1.69	H γ 0.06, -0.21; γ CH ₃ 0.59; δ CH ₃ -1.26
Gly	77	7.23	4.31, 3.97		
Glu	78	8.97	5.01	1.63	H γ 2.08
Leu	79	8.62	4.48	2.07	H γ 1.61; δ CH ₃ 0.89, 0.60
His	80	8.97	3.70	2.78, 2.50	H δ 2 6.90; H ϵ 1 7.51
Pro	81		3.65	2.10, 1.66	H γ 1.32, 1.47; H δ 2.20
Asp	82	10.96	4.39	2.56, 2.62	
Asp	83	8.11	4.83	2.85, 2.56	
Arg	84	7.28	4.19	2.55, 1.67	
Ser	85	7.82	4.37		
Lys	86	7.62	4.19	2.96, 1.82	H γ 1.35
Ile	87	7.28	4.22	1.95	H γ 1.16, 0.83; δ CH ₃ 1.34
Ala	88	7.81	4.24	1.32	
Lys	89	8.30	4.58	1.80	H γ 1.69, 1.67
Pro	90				
Ser	91	8.44	4.41	3.84	

Glu	92	7.82	4.11	1.67	γCH_3 2.95
Thr	93				
Leu	94				

Heme proton chemical shifts (ppm)

8-CH₃ 2.76, 5-CH₃ 19.85, 1-CH₃ 10.28, 3-CH₃ 14.58, 2-HC α 27.34, 2-HC β (trans) -7.08, 2-HC β (cis) -7.5, 4-HC α 4.34, 4-HC β (trans) 2.83, 4-HC β (cis) 2.54, 7-H α 19.55, 7-H α' -1.32, 7-H β 1.63, 7-H β' -3.86, 6-H α 15.33, 6-H α' 14.33, 6-H β -0.76, 6-H β' -1.69, α -meso -3.26, β -meso 9.21, γ -meso -0.71

Experimental NOE intensity

An asterisk indicates the intensity of peaks corresponding to two or more protons with degenerate chemical shifts, which are divided by the number of degenerate protons. Upper distance limits (Å) are also given.

154 LHEM

FE	39 HIS NE2	2.10	3.00e+00
FE	63 HIS NE2	2.10	3.00e+00
FE	124 LTNS PCN	0.20	5.00e+00

2 LYS+

HN	2 LYS+ HA	3.90	26640.0
HN	2 LYS+ QB	5.20	9820.0*2
HN	2 LYS+ QG	5.70	14860.0*2
HN	2 LYS+ QD	5.40	21065.0*2
HA	2 LYS+ QG	6.10	5300.0*2
HA	2 LYS+ QE	6.30	8285.0*2
HA	3 ASP- HN	4.70	8692.0

3 ASP-

HN	3 ASP- HA	4.80	7319.0
HN	3 ASP- HB2	4.00	22860.0
HN	3 ASP- HB3	3.70	37950.0
HA	3 ASP- HB2	4.20	17240.0
HA	3 ASP- HB3	3.70	36890.0
HA	4 VAL HN	3.40	57520.0
HB2	4 VAL HN	4.80	7365.0
HB3	4 VAL HN	4.80	7389.0

4 VAL

HN	4 VAL HA	3.60	44500.0
HN	4 VAL HB	3.60	46750.0
HN	4 VAL QG1	4.30	46060.0
HN	4 VAL QG2	4.80	23800.0
HN	5 LYS+ HN	4.00	24320.0
HA	4 VAL HB	3.60	41890.0
HA	4 VAL QG1	3.90	68160.0
HA	4 VAL QG2	4.20	50780.0
HA	5 LYS+ HN	3.30	69180.0
HA	6 TYR HN	5.50	3277.0
HB	4 VAL QG1	3.40	152900.0
HB	4 VAL QG2	3.50	120800.0
HB	5 LYS+ HN	3.00	134700.0
QG1	5 LYS+ HN	4.70	48600.0
QG1	6 TYR CG	7.90	11335.0*2
QG1	6 TYR CZ	7.50	19100.0*2
QG1	78 GLU- QG	6.50	18980.0*2
QG2	5 LYS+ HN	4.80	39750.0
QG2	5 LYS+ HA	6.20	8801.0
QG2	6 TYR CG	7.80	13515.0*2
QG2	6 TYR CZ	6.80	40950.0*2
QG2	78 GLU- HN	5.60	16750.0
QG2	78 GLU- QB	7.30	8000.0*2
QG2	78 GLU- QG	6.20	26355.0*2

5 LYS+

HN	5 LYS+ HA	3.30	71010.0
HN	5 LYS+ QB	3.90	77450.0*2
HN	7 TYR CZ	7.50	5130.0*2
HA	5 LYS+ QB	4.30	70450.0*2

HA	5 LYS+ HG2	5.00	11720.0
HA	5 LYS+ HG3	4.60	16510.0
HA	6 TYR HN	3.00	139300.0
HA	6 TYR HA	4.90	6941.0
HA	6 TYR CG	7.50	5205.0*2
HA	7 TYR CZ	7.50	14065.0*2
HA	77 GLY HA1	3.20	59910.0
QB	6 TYR HN	5.30	15385.0*2
QB	6 TYR HA	6.50	2789.5*2
QB	7 TYR CZ	8.50	18952.5*4
QB	76 ILE QD1	7.50	1822.0*2
QB	77 GLY HA1	6.50	4192.5*2
QB	78 GLU- HN	6.50	8135.0*2
HG2	5 LYS+ HE3	5.00	11110.0
HG2	6 TYR HN	5.50	7406.0
HG3	5 LYS+ HE2	3.80	45000.0
HG3	5 LYS+ HE3	4.90	12280.0
QD	5 LYS+ HE2	5.70	16240.0*2
HE2	76 ILE HA	5.50	7328.0
6 TYR			
HN	6 TYR HA	3.80	31350.0
HN	6 TYR CG	6.60	17665.0*2
HA	6 TYR HB2	3.60	47260.0
HA	6 TYR HB3	3.30	79720.0
HA	6 TYR CG	4.20	101100.0*2
HA	6 TYR CZ	5.80	9540.0*2
HA	7 TYR HN	3.00	148300.0
HA	7 TYR HA	5.30	4400.0
HA	29 VAL QG2	6.50	1710.0
HA	77 GLY HA2	5.50	1408.0
HA	78 GLU- HN	3.50	35290.0
HA	78 GLU- QB	6.50	4270.5*2
HA	80 HIS HA	4.70	5594.0
HA	80 HIS HD2	5.50	7092.0
HB2	6 TYR CG	5.60	55950.0*2
HB2	6 TYR CZ	7.50	6450.0*2
HB2	7 TYR HN	4.50	11380.0
HB2	80 HIS HA	4.80	39860.0
HB2	80 HIS HD2	4.40	67610.0
HB2	81 PRO HG3	5.40	19850.0
HB3	6 TYR CG	5.70	51600.0*2
HB3	6 TYR CZ	7.50	5730.0*2
HB3	80 HIS HA	5.50	16080.0
HB3	80 HIS HD2	4.60	51740.0
CG	6 TYR CZ	7.20	104725.0*4
CG	78 GLU- HN	7.50	9810.0*2
CG	78 GLU- QB	8.50	12027.5*4
CG	78 GLU- QG	8.50	7705.0*4
CG	80 HIS HA	7.00	31120.0*2
CG	81 PRO QD	8.20	24215.0*4
CZ	78 GLU- HN	7.50	3431.0*2
CZ	78 GLU- HA	7.50	1802.5*2
CZ	78 GLU- QB	8.50	10572.5*4
CZ	78 GLU- QG	8.50	9552.5*4
CZ	80 HIS HA	7.50	6735.0*2
CZ	81 PRO HG2	7.50	8120.0*2
CZ	81 PRO HG3	7.50	7575.0*2
CZ	81 PRO QD	8.50	6622.5*4
7 TYR			
HN	7 TYR HA	3.40	63060.0
HN	7 TYR HB2	3.80	34490.0
HN	7 TYR HB3	4.10	18980.0

HN	29 VAL HB	5.00	32220.0	HA	80 HIS HD2	5.50	14290.0
HN	29 VAL QG2	5.70	13990.0	HB	8 THR QG2	3.40	163000.0
HN	80 HIS HN	3.30	47530.0	HB	9 LEU HN	3.70	36580.0
HN	80 HIS HD2	5.50	2604.0	HB	10 GLU- HN	4.30	22720.0
HA	7 TYR HB2	3.50	53530.0	HB	11 GLU- HN	3.90	44970.0
HA	7 TYR HB3	3.20	90740.0	QG2	9 LEU HN	5.10	28360.0
HA	7 TYR CG	4.60	58650.0*2	QG2	80 HIS HN	6.20	8841.0
HA	8 THR HN	2.80	203300.0	QG2	80 HIS HB2	4.80	38950.0
HA	8 THR QG2	5.40	19600.0	QG2	80 HIS HB3	4.70	47230.0
HA	80 HIS HD2	5.50	4823.0	QG2	80 HIS HD2	4.60	57120.0
HB2	7 TYR CG	5.40	75750.0*2	9 LEU			
HB2	12 ILE HA	5.50	2021.0	HN	9 LEU HA	3.70	36270.0
HB2	12 ILE HG13	5.00	31540.0	HN	9 LEU HB2	3.50	54090.0
HB2	22 TRP HE3	5.50	6506.0	HN	9 LEU HB3	3.30	76320.0
HB2	22 TRP HZ3	5.50	9857.0	HN	9 LEU HG	4.00	35770.0
HB2	29 VAL QG1	6.00	10910.0	HN	9 LEU QD1	4.60	32660.0
HB2	29 VAL QG2	5.10	28700.0	HN	9 LEU QD2	4.70	27710.0
HB2	76 ILE QD1	6.50	1404.0	HN	10 GLU- HN	3.70	35640.0
HB2	79 LEU QD1	6.40	7505.0	HN	11 GLU- HN	5.50	4464.0
HB3	7 TYR CG	5.60	55550.0*2	HN	12 ILE HG13	5.50	4245.0
HB3	12 ILE HA	5.50	4708.0	HN	80 HIS HN	5.50	1116.0
HB3	12 ILE HG12	5.20	26190.0	HN	80 HIS HB3	5.10	28110.0
HB3	12 ILE HG13	4.90	34670.0	HN	83 ASP- HB2	5.50	7098.0
HB3	22 TRP HE3	5.50	7423.0	HN	83 ASP- HB3	5.50	7270.0
HB3	22 TRP HZ3	5.30	22350.0	HA	9 LEU HB2	3.60	44830.0
HB3	29 VAL QG1	6.50	5698.0	HA	9 LEU HB3	3.50	49500.0
HB3	29 VAL QG2	5.40	20640.0	HA	9 LEU HG	3.90	37890.0
HB3	79 LEU QD1	6.10	9359.0	HA	9 LEU QD1	3.40 <	174300.0
CG	7 TYR CZ	7.40	76125.0*4	HA	9 LEU QD2	4.00 >	59890.0
CG	8 THR HN	7.50	14195.0*2	HA	10 GLU- HN	4.30	15390.0
CG	11 GLU- QG	8.50	12645.0*4	HA	12 ILE HB	3.40	92810.0
CG	12 ILE HG13	7.50	10870.0*2	HB2	10 GLU- HN	3.70 <	40460.0
CG	22 TRP HZ3	7.30	23695.0*2	HB3	9 LEU QD1	3.40	135000.0
CG	22 TRP HH2	7.30	22930.0*2	HB3	10 GLU- HN	4.30 >	14740.0
CG	29 VAL HB	7.20	26000.0*2	HG	9 LEU QD1	3.40	361300.0
CG	29 VAL QG1	7.80	13325.0*2	HG	83 ASP- HB2	5.50	7615.0
CG	29 VAL QG2	7.00	31100.0*2	QD1	52 GLY HA1	6.50	5649.0
CG	76 ILE HG13	7.50	580.0*2	QD1	83 ASP- HB2	5.40	19860.0
CG	76 ILE QD1	8.50	4224.0*2	QD1	83 ASP- HB3	4.80	42730.0
CG	77 GLY HA1	7.40	19275.0*2	QD2	83 ASP- HB2	4.60	50230.0
CG	77 GLY HA2	7.50	10415.0*2	QD2	83 ASP- HB3	4.50	60530.0
CG	78 GLU- HN	7.50	9450.0*2	10 GLU-			
CZ	22 TRP HZ3	7.50	9080.0*2	HN	10 GLU- HA	3.30	74560.0
CZ	29 VAL QG1	8.50	1444.5*2	HN	10 GLU- HB2	3.50	51400.0
CZ	76 ILE HG13	7.50	7545.0*2	HN	10 GLU- HB3	3.80	30490.0
CZ	76 ILE QD1	7.70	14805.0*2	HN	10 GLU- HG2	4.80	14160.0
CZ	77 GLY HA1	7.10 <	28605.0*2	HN	10 GLU- HG3	4.10	31350.0
CZ	77 GLY HA2	7.50 >	6600.0*2	HN	11 GLU- HN	3.80	34170.0
CZ	78 GLU- HN	7.50	4895.0*2	HA	10 GLU- HB2	3.10 <	118800.0
8 THR				HA	10 GLU- HB3	3.80 >	30610.0
HN	8 THR HA	3.60	46440.0	HA	10 GLU- HB3	3.80 >	30610.0
HN	8 THR QG2	3.40	144800.0	HA	10 GLU- HG2	3.70	49710.0
HN	9 LEU HN	5.40	3750.0	HA	10 GLU- HG3	4.50	20260.0
HN	11 GLU- HN	5.00	9274.0	HA	13 GLN HN	5.10	8536.0
HN	11 GLU- HB2	3.90	43270.0	HA	13 GLN HB3	3.70	59710.0
HN	11 GLU- HB3	3.80	52120.0	HA	13 GLN QG	6.50	6045.0*2
HN	12 ILE HG13	5.50	3572.0	HB2	10 GLU- HG2	3.20	101600.0
HN	80 HIS HD2	5.50	4428.0	HB2	11 GLU- HN	3.60 <	45740.0
HA	8 THR QG2	3.50	121900.0	HB3	11 GLU- HN	4.60 >	10490.0
HA	9 LEU HN	3.20	95230.0	HG2	14 LYS+ QE	6.50	16835.0*2
HA	80 HIS HN	3.00	80380.0	HG3	11 GLU- HN	5.50	9286.0
HA	80 HIS HB2	4.60	54170.0	11 GLU-			
				HN	11 GLU- HA	3.50	49070.0

HN	11 GLU- HB2	3.10	119900.0	HN	13 GLN QG	4.50	72450.0*2
HN	11 GLU- HB3	3.00	141100.0	HN	14 LYS+ HN	3.40	57490.0
HN	11 GLU- QG	6.30	8300.0*2	HN	15 HIS HD2	5.50	4844.0
HN	12 ILE HN	3.50	52820.0	HA	13 GLN HB2	3.80	31630.0
HN	12 ILE HG13	5.50	3715.0	HA	13 GLN HB3	3.40	63730.0
HA	11 GLU- HB2	3.30	71580.0	HA	13 GLN QG	4.20	62350.0*2
HA	11 GLU- HB3	3.30	74950.0	HA	14 LYS+ HN	3.90	27900.0
HA	11 GLU- QG	6.10	2744.0*2	HA	15 HIS HN	4.40	21110.0
HA	12 ILE HN	4.50	10720.0	HA	51 GLY HA1	4.00	13510.0
HA	14 LYS+ QE	6.50	14285.0*2	HA	51 GLY HA2	3.60	26140.0
HB2	11 GLU- QG	5.10 >	32030.0*2	HB2	13 GLN QG	4.40	82450.0*2
HB2	12 ILE HN	4.10	19440.0	HB2	14 LYS+ HN	4.50	11230.0
HB3	11 GLU- QG	4.30 <	89100.0*2	HB3	13 GLN QG	4.20	105700.0*2
HB3	12 ILE HN	3.60	41440.0	HB3	14 LYS+ HN	4.00	22190.0
QG	15 HIS HD2	6.50	3817.0*2	QG	14 LYS+ HN	6.50	3840.0*2
QG	22 TRP HZ3	6.50	8660.0*2	QG	51 GLY HA2	6.50	5690.0*2
QG	22 TRP HH2	6.50	3532.5*2	14 LYS+			
12 ILE				HN	14 LYS+ HA	3.20	96820.0
HN	12 ILE HA	3.50	54140.0	HN	14 LYS+ QB	4.00	68400.0*2
HN	12 ILE HB	3.10	104000.0	HN	14 LYS+ QG	5.40	21260.0*2
HN	12 ILE QG2	5.80	9604.0	HN	14 LYS+ QD	4.50	65200.0*2
HN	12 ILE HG12	3.50	71350.0	HN	14 LYS+ QE	6.50	1751.0*2
HN	12 ILE HG13	3.30	97450.0	HN	15 HIS HN	3.00	139200.0
HN	13 GLN HN	3.20	89930.0	HN	15 HIS HB2	4.30	15850.0
HN	14 LYS+ HN	5.50	1119.0	HA	14 LYS+ QB	4.70	37330.0*2
HA	12 ILE HB	3.80	30280.0	HA	14 LYS+ QG	4.10	64600.0*2
HA	12 ILE QG2	3.90	68400.0	HA	14 LYS+ QD	4.30	97500.0*2
HA	12 ILE HG12	3.90 >	37710.0	HA	15 HIS HN	4.00	24090.0
HA	12 ILE HG13	3.20 <	103000.0	QB	14 LYS+ QE	7.50	3260.0*4
HA	13 GLN HN	5.00	6266.0	QB	15 HIS HN	5.70	9350.0*2
HA	14 LYS+ HN	4.50	16850.0	QG	14 LYS+ QE	6.40	20380.0*4
HA	15 HIS HN	4.50	16920.0	QG	15 HIS HD2	6.50	17575.0*2
HA	15 HIS HB3	5.50	3841.0	QD	14 LYS+ QE	5.70	52600.0*4
HA	15 HIS HD2	4.10	110400.0	15 HIS			
HA	22 TRP HE3	4.60	54730.0	HN	15 HIS HA	3.70	38900.0
HA	22 TRP HZ3	5.50	18640.0	HN	15 HIS HB2	3.90	26660.0
HA	29 VAL QG1	6.10	9343.0	HN	15 HIS HB3	3.60	40780.0
HA	29 VAL QG2	6.50	4589.0	HN	15 HIS HD2	3.40	80030.0
HB	12 ILE HG13	3.30	99640.0	HN	51 GLY HA2	4.20	11000.0
QG2	12 ILE HG12	3.80	86920.0	HA	15 HIS HB2	3.30	71160.0
QG2	12 ILE HG13	3.60	104800.0	HA	15 HIS HB3	3.70	38450.0
QG2	13 GLN HN	4.90	37110.0	HA	15 HIS HD2	5.20	8844.0
QG2	22 TRP HE3	4.10	114100.0	HA	15 HIS HE1	5.50	1283.0
QG2	22 TRP HZ3	5.10	30210.0	HA	16 LYS+ HN	2.80	207400.0
QG2	29 VAL QG1	5.40	68100.0	HA	17 ASP- HN	5.30	6576.0
QG2	29 VAL QG2	5.80	39930.0	HA	20 SER HB3	5.50	17160.0
HG12	22 TRP HE3	4.40	70150.0	HB2	15 HIS HD2	3.90	40620.0
HG12	22 TRP HZ3	5.20	25200.0	HB2	15 HIS HE1	5.50	2245.0
HG12	29 VAL QG1	5.40	20570.0	HB3	15 HIS HD2	4.20	26490.0
HG12	29 VAL QG2	6.50	2541.0	HB3	15 HIS HE1	5.50	1122.0
HG12	76 ILE QD1	6.50	2087.0	HB3	22 TRP HN	5.20	25870.0
HG13	15 HIS HD2	5.50	13260.0	HD2	15 HIS HE1	5.50	4586.0
HG13	22 TRP HB3	5.50	15540.0	HE1	22 TRP HE1	5.50	5779.0
HG13	22 TRP HE3	4.50	65030.0	HE1	22 TRP HZ2	5.50	14200.0
HG13	22 TRP HZ3	5.00	31260.0	16 LYS+			
HG13	29 VAL QG1	4.50	65120.0	HN	16 LYS+ HA	3.30	75240.0
HG13	29 VAL QG2	4.30	76700.0	HN	16 LYS+ QB	4.80	17050.0*2
HG13	51 GLY HA2	5.50	10910.0	HN	16 LYS+ QG	4.60	58500.0*2
13 GLN				HN	16 LYS+ QD	6.30	8620.0*2
HN	13 GLN HA	3.50	54490.0	HN	17 ASP- HN	3.20	89690.0
HN	13 GLN HB2	3.10	112700.0	HA	16 LYS+ QB	4.00	139000.0*2
HN	13 GLN HB3	3.10	111600.0	HA	16 LYS+ QG	4.80	27110.0*2

HA	16 LYS+ QD	5.10	31020.0*2	QG2	36 LEU QD2	4.60	238800.0
HA	17 ASP- HN	3.70	36540.0	QG2	50 ALA QB	4.70	196700.0
HA	50 ALA QB	3.90	152300.0	QG2	51 GLY HN	5.80	12950.0
HA	51 GLY HN	5.00	3693.0	22 TRP			
QB	16 LYS+ QG	5.70	48900.0*4	HN	22 TRP HA	3.90	29030.0
QB	16 LYS+ QD	5.50	63925.0*4	HN	22 TRP HB2	4.30 <	14150.0
QB	16 LYS+ QE	7.50	6892.5*4	HN	22 TRP HB3	5.10 >	5448.0
QB	51 GLY HA1	6.50	4730.5*2	HN	22 TRP HD1	4.80	14010.0
QB	51 GLY HA2	6.50	4379.5*2	HN	50 ALA QB	6.10	9429.0
QG	16 LYS+ QD	5.90	37225.0*4	HN	51 GLY HN	3.90	18190.0
QG	16 LYS+ QE	6.60	16797.5*4	HA	22 TRP HB2	3.90 >	28740.0
QD	16 LYS+ QE	7.40	7565.0*4	HA	22 TRP HB3	3.30 <	76020.0
17 ASP-				HA	22 TRP HD1	3.70	53760.0
HN	17 ASP- HA	3.90	27640.0	HA	22 TRP HE3	4.70	15140.0
HN	17 ASP- HB2	4.80	8116.0	HA	22 TRP HE1	4.80	14510.0
HN	17 ASP- HB3	4.20	16180.0	HA	23 VAL HN	3.00	132500.0
HA	17 ASP- HB2	3.30	73680.0	HA	23 VAL QG1	5.80	13400.0
HA	17 ASP- HB3	3.70	38850.0	HA	23 VAL QG2	5.90	11560.0
19 LYS+				HA	29 VAL QG1	6.00	10220.0
HN	19 LYS+ HA	3.40	63440.0	HA	31 ASP- HA	3.10	62750.0
HN	19 LYS+ QB	4.00	64100.0*2	HA	32 LEU HN	3.20	53010.0
HN	19 LYS+ QG	5.40	21040.0*2	HA	32 LEU QD1	6.50	4177.0
HN	19 LYS+ QD	5.80	14295.0*2	HA	76 ILE QD1	6.50	2047.0
HN	20 SER HN	2.80	207400.0	HB2	22 TRP HE3	4.50	20260.0
HA	19 LYS+ QB	4.50	50500.0*2	HB2	23 VAL HN	3.80	29490.0
HA	19 LYS+ QG	5.00	21105.0*2	HB2	29 VAL QG1	5.40	19660.0
HA	19 LYS+ QD	6.20	9570.0*2	HB3	22 TRP HD1	4.90	12020.0
HA	20 SER HN	3.60	42070.0	HB3	22 TRP HE3	4.10	31770.0
QB	19 LYS+ QG	6.00	36925.0*4	HB3	23 VAL HN	3.80	34560.0
QB	19 LYS+ QE	7.50	1233.8*4	HB3	29 VAL QG1	4.80	42800.0
QB	20 SER HN	4.70	37930.0*2	HB3	76 ILE QD1	6.50	2389.0
QG	19 LYS+ QD	5.80	48175.0*4	HD1	22 TRP HE1	3.60	62520.0
QG	19 LYS+ QE	6.50	18550.0*4	HD1	23 VAL HN	5.50	14280.0
20 SER				HD1	31 ASP- HA	4.10	104200.0
HN	20 SER HA	3.30	69210.0	HD1	32 LEU HN	4.40	67390.0
HN	20 SER HB2	4.10	21080.0	HD1	76 ILE QD1	6.30	7719.0
HN	20 SER HB3	4.00	24350.0	HE3	22 TRP HZ3	3.70	52590.0
HN	21 THR HN	4.20	17860.0	HE3	29 VAL QG1	4.60 <	57110.0
HN	33 THR QG2	5.10	27360.0	HE3	29 VAL QG2	5.90 >	11630.0
HA	20 SER HB2	3.50	55630.0	HE3	76 ILE HG13	5.50	1267.0
HA	20 SER HB3	3.60	48060.0	HE3	76 ILE QD1	6.10	9642.0
HA	21 THR HN	2.90	177500.0	HE1	22 TRP HZ2	3.70	53300.0
HA	33 THR HA	4.70	5652.0	HE1	31 ASP- HB2	5.50	6479.0
HA	33 THR QG2	4.30	78150.0	HE1	76 ILE QD1	5.50	18340.0
21 THR				HZ3	22 TRP HZ2	4.80	13750.0
HN	21 THR HA	3.70	37160.0	HZ3	22 TRP HH2	3.30	91380.0
HN	21 THR HB	3.50	50310.0	HZ3	29 VAL QG1	5.70 <	13980.0
HN	21 THR QG2	4.30	41200.0	HZ3	29 VAL QG2	6.50 >	2962.0
HN	22 TRP HD1	5.20	24380.0	HZ3	76 ILE QD1	6.50	5581.0
HN	33 THR HA	3.30	47870.0	HZ2	22 TRP HH2	3.10	136500.0
HA	21 THR HB	4.60	10030.0	HZ2	29 VAL QG1	6.50	2497.0
HA	21 THR QG2	4.00	60510.0	HZ2	76 ILE HG13	5.50	369.0
HA	22 TRP HN	3.20	85250.0	HZ2	76 ILE QD1	4.70	47740.0
HA	50 ALA QB	6.00	10810.0	HH2	29 VAL QG1	6.50	2081.0
HB	21 THR QG2	3.40	166100.0	HH2	76 ILE QD1	5.30	21470.0
HB	36 LEU QD1	5.20	26090.0	23 VAL			
HB	36 LEU QD2	5.20	24830.0	HN	23 VAL HA	3.30	74800.0
HB	50 ALA QB	6.50	4466.0	HN	23 VAL HB	4.30	15080.0
QG2	22 TRP HN	4.80	42900.0	HN	23 VAL QG1	4.70	27020.0
QG2	22 TRP HA	5.40	21250.0	HN	23 VAL QG2	4.10	53150.0
QG2	23 VAL QG1	4.90	144300.0	HN	29 VAL QG1	6.00	10300.0
QG2	23 VAL QG2	5.50	64990.0	HN	30 TYR HN	3.40	36590.0

HN	30 TYR HB2	5.00	32210.0
HN	30 TYR CG	7.50	6015.0*2
HN	31 ASP- HA	4.30	9734.0
HN	32 LEU QD1	6.50	1195.0
HA	23 VAL HB	3.30	80430.0
HA	23 VAL QG1	3.90 <	75240.0
HA	23 VAL QG2	4.90 >	23680.0
HA	24 ILE HN	3.10	113900.0
HA	52 GLY HN	3.80	18630.0
HB	23 VAL QG1	3.40	141700.0
HB	23 VAL QG2	3.40	138200.0
HB	24 ILE HN	3.50	53060.0
QG1	24 ILE HN	5.70	14640.0
QG1	25 LEU QD1	6.60	16910.0
QG1	25 LEU QD2	5.80	40190.0
QG1	30 TYR HB2	6.50	5658.0
QG1	30 TYR CG	8.40	7210.0*2
QG1	32 LEU HN	6.50	1809.0
QG1	32 LEU QD1	5.30	81000.0
QG1	49 GLN HN	6.50	4416.0
QG1	49 GLN HB2	5.60	15750.0
QG1	50 ALA HN	5.30 <	23310.0
QG1	50 ALA QB	6.00 <	31690.0
QG1	51 GLY HN	5.10 <	27240.0
QG1	51 GLY HA1	5.70	14980.0
QG1	52 GLY HN	5.80	13610.0
QG1	54 ALA QB	5.00	124000.0
QG1	154 LHEM HV2A	6.20	8546.0
QG2	24 ILE HN	5.70	15130.0
QG2	25 LEU HG	5.30	22870.0
QG2	25 LEU QD1	6.10	27160.0
QG2	25 LEU QD2	5.60	51420.0
QG2	30 TYR HN	5.90	12160.0
QG2	30 TYR HB2	4.30	85150.0
QG2	30 TYR HB3	5.00	31230.0
QG2	30 TYR CG	7.50	17495.0*2
QG2	30 TYR CZ	8.50	3020.5*2
QG2	32 LEU HN	6.50	1891.0
QG2	32 LEU QD1	5.20	96380.0
QG2	32 LEU QD2	5.80	43410.0
QG2	50 ALA HN	6.50 >	2781.0
QG2	50 ALA QB	7.10 >	9903.0
QG2	51 GLY HN	6.50 >	3325.0
QG2	54 ALA QB	5.50	61110.0
QG2	154 LHEM HV2T	6.50	6586.5
QG2	154 LHEM HV2C	6.50	1244.2

24 ILE

HN	24 ILE HA	4.00	24900.0
HN	24 ILE HB	3.70	37110.0
HN	24 ILE HG12	5.10	10150.0
HN	24 ILE HG13	4.60	17130.0
HN	25 LEU HN	5.20	4563.0
HN	29 VAL QG2	6.50	1397.0
HN	52 GLY HN	4.70	5380.0
HN	52 GLY HA1	5.50	1754.0
HN	54 ALA HN	3.80	20090.0
HN	54 ALA QB	6.30	7711.0
HA	24 ILE HB	4.50	11420.0
HA	24 ILE HG12	3.40 <	79770.0
HA	24 ILE HG13	4.20 >	27890.0
HA	25 LEU HN	3.00	125300.0
HA	25 LEU HG	5.50	4204.0

HA	29 VAL HA	3.40	38610.0
HA	29 VAL QG1	6.00	11220.0
HA	29 VAL QG2	5.50	19100.0
HA	30 TYR HN	3.30	49920.0
HA	30 TYR CG	7.50	13975.0*2
HA	30 TYR CZ	7.50	6170.0*2
HB	24 ILE HG12	3.20 <	110700.0
HB	24 ILE HG13	4.30 >	23790.0
HB	25 LEU HN	4.60	9861.0
HB	30 TYR CG	7.50	17315.0*2
HB	54 ALA HN	5.50	14320.0
HG12	26 HIS HN	5.50	3282.0
HG12	29 VAL HA	5.50	3746.0
HG12	29 VAL QG1	6.20	8682.0
HG12	54 ALA HA	5.50	9793.0
HG13	29 VAL QG1	6.50	6871.0
HG13	53 ASP- HA	5.50	1463.0

25 LEU

HN	25 LEU HA	3.60	43610.0
HN	25 LEU HB2	4.50	11480.0
HN	25 LEU HB3	4.80	7856.0
HN	25 LEU HG	4.70	16120.0
HN	25 LEU QD1	5.90	8747.0
HN	25 LEU QD2	6.20	7005.0
HN	26 HIS HN	5.40	3599.0
HN	28 LYS+ HN	4.70	14160.0
HN	30 TYR CG	7.20	24995.0*2
HN	30 TYR CZ	7.10	27570.0*2
HA	25 LEU HB2	4.40 >	13500.0
HA	25 LEU HB3	3.20 <	83420.0
HA	25 LEU HG	4.00	35810.0
HA	25 LEU QD1	6.50 >	3987.0
HA	25 LEU QD2	3.60 <	102400.0
HA	26 HIS HN	3.20	91680.0
HA	55 THR HA	3.50	31680.0
HA	55 THR QG2	5.60	15740.0
HB2	25 LEU HG	3.40	80870.0
HB2	25 LEU QD1	3.50	115800.0
HB2	25 LEU QD2	4.30	43970.0
HB2	26 HIS HD2	5.50	14190.0
HB2	30 TYR CG	7.00	31165.0*2
HB2	30 TYR CZ	6.70	48250.0*2
HB2	55 THR HA	5.50	11870.0
HB3	25 LEU HG	3.30	99960.0
HB3	25 LEU QD1	3.60	104600.0
HB3	25 LEU QD2	3.80	83210.0
HB3	26 HIS HN	4.30	15060.0
HB3	26 HIS HD2	5.10	29700.0
HB3	30 TYR CG	7.50	15670.0*2
HB3	30 TYR CZ	6.90	35125.0*2
HB3	55 THR HA	5.50	9792.0
HG	25 LEU QD1	3.40	281455.8
HG	25 LEU QD2	3.40	150400.0
HG	30 TYR CG	7.30	21640.0*2
HG	30 TYR CZ	7.50	13430.0*2
QD1	26 HIS HN	6.50 >	1180.0
QD1	26 HIS HD2	6.20	8983.0
QD1	30 TYR HB2	6.20	8448.0
QD1	30 TYR CG	7.40 <	19230.0*2
QD1	30 TYR CZ	7.20 <	26130.0*2
QD1	54 ALA HN	6.50 >	993.0
QD1	54 ALA QB	6.90 >	12170.0

QD1	55 THR HN	6.50 >	750.0
QD1	55 THR HA	6.10 >	9674.0
QD1	55 THR QG2	7.50 >	3030.0
QD1	154 LHEM HV2A	4.50	61831.2
QD1	154 LHEM HV2T	4.30	75453.1
QD1	154 LHEM HV2C	4.50	61641.0
QD1	154 LHEM QM3	4.60	56466.2
QD1	71 SER HA	6.50	3712.0
QD1	71 SER QB	7.50	3493.0*2
QD2	26 HIS HN	5.70 <	14310.0
QD2	26 HIS HD2	6.20	8518.0
QD2	30 TYR CG	8.50 >	4993.0*2
QD2	30 TYR CZ	8.50 >	6720.0*2
QD2	54 ALA HN	5.20 <	24760.0
QD2	54 ALA QB	4.90 <	145300.0
QD2	55 THR HN	5.10 <	29200.0
QD2	55 THR HA	4.20 <	87310.0
QD2	55 THR HB	6.30	8092.0
QD2	55 THR QG2	6.40 <	19820.0
QD2	57 ASN HN	6.50	1414.0
QD2	58 PHE HN	5.40	19920.0
QD2	58 PHE HB2	4.40	65830.0
QD2	59 GLU- HN	6.50	6846.0
QD2	154 LHEM HV2A	5.00	31414.1
QD2	154 LHEM QM3	4.10	108252.2
26 HIS			
HN	26 HIS HA	3.30	81980.0
HN	26 HIS QB	5.10	12220.0*2
HN	26 HIS HD2	5.50	4797.0
HN	27 HIS HN	4.90	6760.0
HN	28 LYS+ HN	5.50	1425.0
HN	55 THR HN	4.60	6521.0
HN	55 THR HA	4.30	8883.0
HN	55 THR QG2	4.40	65660.0
HA	26 HIS QB	4.50	55950.0*2
HA	26 HIS HD2	5.50	3598.0
HA	27 HIS HN	3.60	41720.0
QB	26 HIS HD2	4.90	38815.0*2
QB	27 HIS HN	6.50	1502.0*2
QB	28 LYS+ HN	6.50	1117.0*2
QB	55 THR QG2	6.30	22135.0*2
HD2	26 HIS HE1	5.50	1973.0
HD2	55 THR HA	5.50	1903.0
HD2	55 THR QG2	5.10	29190.0
HE1	55 THR QG2	5.50	17290.0
HE1	59 GLU- HG2	5.50	9751.0
HE1	59 GLU- HG3	5.50	12750.0
27 HIS			
HN	27 HIS HA	3.60	43390.0
HN	27 HIS HB2	3.80	32580.0
HN	27 HIS HB3	4.20	16170.0
HN	27 HIS HD2	4.90	13080.0
HN	28 LYS+ HN	4.00	24470.0
HA	27 HIS HB3	3.30	70120.0
HA	27 HIS HD2	5.50	6495.0
HA	28 LYS+ HN	4.00	23050.0
HA	79 LEU HN	4.10	12700.0
HA	79 LEU QB	6.50	1088.5*2
HA	79 LEU HG	5.50	1214.0
HB2	28 LYS+ HN	5.50	1497.0
HB3	27 HIS HD2	4.70	15670.0
HB3	28 LYS+ HN	5.50	2751.0

HD2	27 HIS HE1	5.50	650.0
HE1	87 ILE HB	5.50	16660.0
HE1	87 ILE HG12	5.10	29130.0
HE1	87 ILE HG13	5.20	24640.0
28 LYS+			
HN	28 LYS+ HA	3.90	26070.0
HN	28 LYS+ QB	5.00	12625.0*2
HN	28 LYS+ QG	5.90	12825.0*2
HN	28 LYS+ QD	6.50	2606.0*2
HN	30 TYR CG	7.50	1287.0*2
HN	30 TYR CZ	7.50	7940.0*2
HN	78 GLU- HA	5.30	2598.0
HA	28 LYS+ QB	5.30	14175.0*2
HA	29 VAL HN	3.30	76650.0
HA	29 VAL QG2	5.20	24830.0
HA	78 GLU- HA	4.70	5492.0
HA	78 GLU- QG	6.50	12755.0*2
QB	28 LYS+ QG	7.00	10755.0*4
QB	28 LYS+ QD	5.80	45250.0*4
QB	29 VAL HN	5.80	7315.0*2
QG	28 LYS+ QD	6.90	12972.5*4
QG	28 LYS+ QE	6.60	16582.5*4
QG	29 VAL HN	6.50	4422.0*2
QD	28 LYS+ QE	7.50	2725.0*4
29 VAL			
HN	29 VAL HA	4.90	7116.0
HN	29 VAL HB	3.50	51010.0
HN	29 VAL QG1	4.80	23780.0
HN	29 VAL QG2	4.10	57070.0
HN	30 TYR HN	5.10	5414.0
HN	77 GLY HN	3.90	15820.0
HN	78 GLU- HA	3.30	45240.0
HA	29 VAL HB	3.80	30330.0
HA	29 VAL QG1	3.90	68540.0
HA	29 VAL QG2	4.00	61880.0
HA	30 TYR HN	3.00	142500.0
HA	30 TYR CG	7.10	27750.0*2
HB	29 VAL QG1	3.40	142000.0
HB	29 VAL QG2	3.40	208500.0
HB	30 TYR HN	4.60	9809.0
HB	76 ILE HG13	4.90	34670.0
HB	76 ILE QD1	5.80	13650.0
HB	77 GLY HN	5.50	18590.0
HB	78 GLU- HA	5.50	11030.0
QG1	30 TYR HN	4.60	52930.0
QG1	30 TYR CG	8.50 <	6250.0*2
QG1	31 ASP- HN	6.50	2822.0
QG1	76 ILE HN	6.50	6729.0
QG1	76 ILE HG12	4.20	99450.0
QG1	76 ILE HG13	4.40	67910.0
QG1	76 ILE QD1	5.20 <	93180.0
QG1	77 GLY HN	6.50	4887.0
QG1	78 GLU- HN	6.50 >	768.0
QG1	78 GLU- HA	6.50 >	4123.0
QG2	30 TYR HN	5.30	22180.0
QG2	30 TYR CG	8.50 >	1294.0*2
QG2	76 ILE QD1	7.30 >	7793.0
QG2	77 GLY HN	6.50	3002.0
QG2	78 GLU- HN	5.60 <	16160.0
QG2	78 GLU- HA	4.90 <	37400.0
QG2	79 LEU HA	5.50	17920.0
30 TYR			

HN	30 TYR HA	3.70	40350.0
HN	30 TYR HB2	3.50	52210.0
HN	30 TYR HB3	3.90	25260.0
HN	30 TYR CG	5.80	47715.0*2
HN	30 TYR CZ	5.80	13590.0*2
HA	30 TYR HB2	3.70	38510.0
HA	30 TYR HB3	3.80	34100.0
HA	30 TYR CG	5.50	19350.0*2
HA	31 ASP- HN	3.20	92810.0
HA	75 ILE HA	3.00	85740.0
HA	75 ILE HB	5.50	15380.0
HA	76 ILE HG12	5.50	18520.0
HB2	30 TYR CG	5.80	46670.0*2
HB2	30 TYR CZ	6.90	12450.0*2
HB2	32 LEU QD1	5.80	13260.0
HB2	32 LEU QD2	4.80	43850.0
HB2	154 LHEM HV2T	5.40	21212.9
HB3	30 TYR CG	5.50	64300.0*2
HB3	30 TYR CZ	6.70	15010.0*2
HB3	31 ASP- HN	3.80	31400.0
HB3	32 LEU QD1	5.50	18760.0
HB3	32 LEU QD2	4.20	89610.0
HB3	74 TYR HB2	4.50	59400.0
CG	31 ASP- HN	7.50	4308.5*2
CG	32 LEU HG	7.50	2989.0*2
CG	32 LEU QD1	8.50 >	3567.5*2
CG	32 LEU QD2	6.80 <	39310.0*2
CG	154 LHEM HV2A	7.50	2969.8*2
CG	154 LHEM HV2T	7.00	32913.2*2
CG	154 LHEM HV2C	7.50	7958.2*2
CG	71 SER HA	7.50	14305.0*2
CG	71 SER QB	8.50	8162.5*4
CG	72 LYS+ HN	7.50	2988.5*2
CG	74 TYR HN	6.20	90050.0*2
CG	74 TYR HA	7.50	6635.0*2
CG	74 TYR HB2	6.60	54050.0*2
CG	74 TYR HB3	7.30	23070.0*2
CG	74 TYR CG	9.50	17457.5*4
CG	75 ILE HN	7.50	10695.0*2
CG	75 ILE HA	7.50	12420.0*2
CG	75 ILE HG13	7.50	3301.0*2
CG	75 ILE QD1	8.00	10240.0*2
CG	76 ILE HN	7.50	2521.0*2
CZ	154 LHEM HV2A	7.50	3489.2*2
CZ	154 LHEM HV2T	7.50	18926.1*2
CZ	154 LHEM HV2C	7.50	5583.8*2
CZ	71 SER HA	7.20	25560.0*2
CZ	71 SER QB	8.50	10237.5*4
CZ	72 LYS+ HN	7.50	2285.0*2
CZ	72 LYS+ HA	7.50	13490.0*2
CZ	74 TYR HN	7.50	7350.0*2
CZ	74 TYR HB2	7.30	23395.0*2
CZ	74 TYR HB3	7.50	11260.0*2
CZ	74 TYR CG	8.80	41475.0*4
CZ	75 ILE HN	7.50	9635.0*2
CZ	75 ILE HA	7.50	12840.0*2
CZ	75 ILE HB	6.80	41040.0*2
CZ	75 ILE QG2	8.30	8260.0*2
CZ	75 ILE HG12	6.90 <	36140.0*2
CZ	75 ILE HG13	7.50 >	3045.5*2
CZ	75 ILE QD1	7.80	13215.0*2

31 ASP-

HN	31 ASP- HA	4.30	14900.0
HN	31 ASP- HB2	3.50	55660.0
HN	31 ASP- HB3	3.60	45560.0
HN	32 LEU QD2	6.00	10300.0
HN	74 TYR HB2	5.50	5055.0
HN	74 TYR HB3	5.50	10750.0
HN	74 TYR CG	7.50	1354.5*2
HN	75 ILE HA	4.30	8773.0
HN	76 ILE HN	4.00	15330.0
HN	76 ILE QG2	4.60	51070.0
HN	76 ILE HG12	5.50	4426.0
HN	76 ILE HG13	5.50	2628.0
HN	76 ILE QD1	5.80	12740.0
HA	31 ASP- HB2	3.40	64150.0
HA	31 ASP- HB3	3.50	49220.0
HA	32 LEU HN	2.90	183200.0
HA	32 LEU HG	5.50	5827.0
HA	76 ILE QG2	6.50	6751.0
HA	76 ILE QD1	5.50	18510.0
HB2	76 ILE HB	4.50	60720.0
HB2	76 ILE QG2	4.50	59610.0
HB2	76 ILE HG12	5.50	10130.0
HB2	76 ILE HG13	5.50	9322.0
HB2	76 ILE QD1	4.20	91940.0
32 LEU			
HN	32 LEU HA	3.80	34210.0
HN	32 LEU QB	5.20	10550.0*2
HN	32 LEU HG	3.40	78320.0
HN	32 LEU QD1	5.10	18000.0
HN	32 LEU QD2	5.20	16730.0
HN	33 THR HN	3.20	94620.0
HN	34 LYS+ HN	5.40	6235.0
HA	32 LEU QB	4.90	27040.0*2
HA	32 LEU HG	4.20	25930.0
HA	32 LEU QD1	5.40 >	14100.0
HA	32 LEU QD2	3.40 <	211800.0
HA	33 THR HN	4.00	22460.0
HA	34 LYS+ HN	4.70	13020.0
HA	35 PHE HN	4.00	34350.0
HA	35 PHE HB2	4.60	15990.0
HA	35 PHE HB3	4.00	38780.0
HA	35 PHE CG	7.50	5970.0*2
HA	74 TYR CG	7.50	9280.0*2
QB	32 LEU HG	4.70	54350.0*2
QB	32 LEU QD1	5.30	45560.0*2
QB	32 LEU QD2	5.50	35010.0*2
QB	33 THR HN	6.50	516.0*2
QB	35 PHE HB3	6.50	7060.0*2
QB	35 PHE CG	8.50	9672.5*4
QB	36 LEU QD2	4.60	247550.0*2
QB	46 LEU HB2	6.00	31990.0*2
HG	32 LEU QD1	3.40	194900.0
HG	32 LEU QD2	3.40	167900.0
HG	154 LHEM HV2T	5.50	11464.5
QD1	35 PHE HB3	6.40	7576.0
QD1	35 PHE CG	7.50	19075.0*2
QD1	36 LEU QD2	6.60	16000.0
QD1	154 LHEM HV2T	4.80 >	40028.6
QD1	154 LHEM HV2C	5.30	23130.6
QD1	74 TYR CG	8.50 >	2706.5*2
QD1	74 TYR CZ	8.50 >	1554.5*2
QD2	33 THR HN	6.50	4218.0

QD2	35 PHE HN	6.30	7693.0
QD2	35 PHE HA	6.50	5350.0
QD2	35 PHE HB2	5.50	17290.0
QD2	35 PHE HB3	4.80	42380.0
QD2	35 PHE CG	6.70	45260.0*2
QD2	154 LHEM HV2A	4.70	45355.6
QD2	154 LHEM HV2T	4.10 <	108290.3
QD2	154 LHEM HV2C	4.80	43034.6
QD2	74 TYR HN	6.00	10490.0
QD2	74 TYR HB2	4.60	52120.0
QD2	74 TYR HB3	4.30	76440.0
QD2	74 TYR CG	7.40 <	19390.0*2
QD2	74 TYR CZ	8.50 <	6625.0*2
33 THR			
HN	33 THR HA	3.20	88670.0
HN	33 THR HB	3.40	64760.0
HN	33 THR QG2	5.00	19570.0
HN	34 LYS+ HN	3.60	45400.0
HN	35 PHE HN	4.60	15810.0
HA	33 THR HB	3.70	38000.0
HA	33 THR QG2	3.40	241000.0
HA	34 LYS+ HN	4.50	11620.0
HA	34 LYS+ HG2	4.50	64190.0
HA	36 LEU HN	5.10	8377.0
HA	36 LEU HB2	5.10	8276.0
HA	36 LEU QD1	4.70	48100.0
HA	36 LEU QD2	5.30	21460.0
HB	33 THR QG2	3.40	258300.0
HB	34 LYS+ HN	3.50	56390.0
QG2	34 LYS+ HN	5.30	23850.0
QG2	34 LYS+ HA	5.60	15850.0
34 LYS+			
HN	34 LYS+ HA	3.40	63920.0
HN	34 LYS+ HB2	3.40	65040.0
HN	34 LYS+ HB3	3.60	46780.0
HN	34 LYS+ HG2	4.10	32730.0
HN	34 LYS+ HG3	4.20	26510.0
HN	34 LYS+ QD	6.50	7275.0*2
HN	35 PHE HN	3.10	119300.0
HN	36 LEU HN	4.80	12470.0
HN	74 TYR CG	7.50	1135.0*2
HN	74 TYR CZ	7.50	3472.5*2
HA	34 LYS+ HB2	3.60	45110.0
HA	34 LYS+ HB3	3.40	65900.0
HA	34 LYS+ HG2	3.90	38680.0
HA	34 LYS+ HG3	3.90	40880.0
HA	34 LYS+ QD	5.70	15755.0*2
HA	35 PHE HN	4.10	20470.0
HA	36 LEU HN	5.50	5103.0
HB2	35 PHE HN	4.10 <	18990.0
HB2	74 TYR CG	7.50	13695.0*2
HB2	74 TYR CZ	7.50	11410.0*2
HB3	34 LYS+ HG2	4.20	28140.0
HB3	34 LYS+ HG3	3.80	48370.0
HB3	34 LYS+ QD	4.90	38500.0*2
HB3	35 PHE HN	5.30 >	4271.0
HB3	74 TYR CZ	7.50	8200.0*2
HG2	34 LYS+ QE	6.50	2692.0*2
HG3	34 LYS+ QE	6.50	3446.5*2
QD	34 LYS+ QE	7.00	11152.5*4
35 PHE			
HN	35 PHE HA	3.30	70880.0

HN	35 PHE HB2	3.30	77700.0
HN	35 PHE HB3	3.00	132300.0
HN	35 PHE CG	6.20	26035.0*2
HN	36 LEU HN	2.80	194800.0
HN	36 LEU HB2	4.70	9201.0
HN	36 LEU HB3	5.40	3755.0
HN	37 GLU- HN	5.50	3955.0
HN	74 TYR CG	7.50	1222.0*2
HN	74 TYR CZ	7.50	3890.0*2
HA	35 PHE HB2	3.00	136400.0
HA	35 PHE HB3	3.30	80490.0
HA	35 PHE CG	4.30	87350.0*2
HA	36 LEU HN	4.10	20540.0
HA	38 GLU- HN	5.00	9805.0
HA	38 GLU- HB2	4.10	32160.0
HA	38 GLU- HB3	3.80	50840.0
HA	38 GLU- HG2	5.50	7487.0
HA	38 GLU- HG3	5.50	13770.0
HA	39 HIS HN	5.00	8890.0
HA	74 TYR CZ	7.50	6995.0*2
HB2	35 PHE CG	5.50	69700.0*2
HB2	36 LEU HN	4.40	13790.0
HB2	74 TYR CG	7.50	8645.0*2
HB2	74 TYR CZ	7.30	22105.0*2
HB3	35 PHE CG	5.60	56350.0*2
HB3	36 LEU HN	4.10	20620.0
HB3	74 TYR CG	7.50	4715.5*2
HB3	74 TYR CZ	7.50	10875.0*2
CG	35 PHE CZ	8.50	18202.5*4
CG	36 LEU HN	7.50	9840.0*2
CG	36 LEU QD2	8.40	7385.0*2
CG	38 GLU- HB2	7.10	29035.0*2
CG	38 GLU- HB3	7.10	29825.0*2
CG	39 HIS HN	7.50	12000.0*2
CG	46 LEU QD1	8.50	6355.0*2
CG	154 LHEM HV2A	7.50	3898.2*2
CG	154 LHEM HV2T	7.50	1371.7*2
CG	154 LHEM HV2C	7.50	2722.5*2
CG	70 LEU QD1	8.50	4685.5*2
CG	74 TYR CZ	9.50	5725.0*4
CZ	35 PHE HZ	6.60	17005.0*2
CZ	39 HIS HN	6.70	47685.0*2
CZ	46 LEU QD1	7.80	12560.0*2
CZ	70 LEU HG	7.50	3477.5*2
CZ	70 LEU QD1	8.10	9550.0*2
CZ	70 LEU QD2	8.50	6810.0*2
HZ	70 LEU QD2	6.40	7184.0
36 LEU			
HN	36 LEU HA	3.30	73460.0
HN	36 LEU HB2	3.10	118200.0
HN	36 LEU HB3	3.50	53200.0
HN	36 LEU HG	3.90	42150.0
HN	36 LEU QD1	4.70	28000.0
HN	36 LEU QD2	4.50	35070.0
HN	37 GLU- HN	3.50	56460.0
HN	38 GLU- HN	4.20	26540.0
HN	43 GLU- HA	5.50	607.0
HA	36 LEU HB3	3.60	41560.0
HA	36 LEU HG	3.30	86080.0
HA	36 LEU QD1	4.70 >	27970.0
HA	36 LEU QD2	3.40 <	201700.0
HA	39 HIS HN	4.50	16980.0

HA	43 GLU- HA	4.00	13640.0
HB2	36 LEU HG	3.10	135300.0
HB2	36 LEU QD1	3.80	80700.0
HB2	36 LEU QD2	4.00	66120.0
HB2	38 GLU- HN	4.90	10930.0
HB2	43 GLU- HA	5.50	8335.0
HB3	36 LEU HG	3.00	145300.0
HB3	36 LEU QD1	3.90	72090.0
HB3	36 LEU QD2	4.20	47540.0
HB3	43 GLU- HA	5.50	10290.0
HB3	43 GLU- HB2	5.50	11780.0
HG	36 LEU QD1	3.90	72090.0
HG	36 LEU QD2	4.00	60970.0
HG	37 GLU- HN	5.50	13300.0
HG	43 GLU- HA	5.50	13660.0
HG	43 GLU- HB2	5.00	33270.0
QD1	43 GLU- HA	6.20 >	9072.0
QD1	43 GLU- HB2	5.80	13010.0
QD1	46 LEU HB2	6.40	7268.0
QD1	47 ARG+ QB	5.30 <	86500.0*2
QD1	47 ARG+ QG	6.80	13585.0*2
QD1	47 ARG+ QD	7.40 <	7350.0*2
QD1	47 ARG+ HE	6.50	6780.0
QD2	43 GLU- HN	6.50	743.0
QD2	43 GLU- HA	5.00 <	31100.0
QD2	43 GLU- HB2	5.20	26000.0
QD2	46 LEU HB2	4.20	99410.0
QD2	47 ARG+ HN	6.50	3693.0
QD2	47 ARG+ HA	6.50	3440.0
QD2	47 ARG+ QB	7.10 >	9790.0*2
QD2	47 ARG+ QG	6.20	24270.0*2
QD2	47 ARG+ QD	7.50 >	2550.0*2
37 GLU-			
HN	37 GLU- HA	3.20	86890.0
HN	37 GLU- HB2	3.40	59420.0
HN	37 GLU- HB3	3.00	143800.0
HN	37 GLU- QG	5.10	29130.0*2
HN	38 GLU- HN	3.20	87140.0
HN	39 HIS HN	4.90	10010.0
HA	37 GLU- HB2	3.20	96750.0
HA	37 GLU- HB3	3.40	59930.0
HA	37 GLU- QG	4.80	28175.0*2
HB3	37 GLU- QG	4.50	64400.0*2
HB3	38 GLU- HN	4.30	14740.0
38 GLU-			
HN	38 GLU- HA	3.20	97170.0
HN	38 GLU- HB2	3.40	58120.0
HN	38 GLU- HB3	3.50	55140.0
HN	38 GLU- HG2	3.60	58670.0
HN	38 GLU- HG3	3.70	50390.0
HN	39 HIS HN	3.10	101700.0
HA	38 GLU- HB2	3.30	82270.0
HA	38 GLU- HB3	3.70	35370.0
HA	38 GLU- HG2	3.50	72930.0
HA	38 GLU- HG3	4.00	37180.0
HA	39 HIS HN	4.00	25020.0
HB2	38 GLU- HG2	2.70	277200.0
HB2	38 GLU- HG3	2.60	283800.0
HB2	39 HIS HN	3.70	35520.0
HB3	38 GLU- HG3	3.20	107800.0
HB3	39 HIS HN	3.80	32140.0
39 HIS			

HN	39 HIS HA	4.20	16320.0
HN	39 HIS HB2	2.90 <	166697.0
HN	39 HIS HB3	3.80 >	33950.0
HN	42 GLY HN	5.50	779.0
HA	39 HIS HB2	3.40	61184.4
HA	40 PRO HG2	5.50	1280.0
HA	40 PRO HG3	5.50	1488.0
HB2	39 HIS HD1	4.60	17765.5
HB2	42 GLY HN	5.50	3903.9
HB2	43 GLU- HA	5.40	6236.4
HB2	46 LEU HB2	4.60	55971.6
HB3	39 HIS HD1	4.30	24660.2
HB3	42 GLY HN	5.50	2857.0
HD1	42 GLY HN	5.50	9828.3
HD1	43 GLU- HA	5.50	7046.9
HD1	45 VAL QG1	6.50	5871.1
HD1	45 VAL QG2	5.80	13789.3
HD1	46 LEU HB2	5.50	11864.0
40 PRO			
HA	40 PRO HB2	3.50	54540.0
HA	40 PRO HB3	3.20	88770.6
HA	40 PRO HG2	4.70	15990.0
HA	40 PRO HG3	5.10	10060.0
HA	42 GLY HN	5.30	6307.0
HB2	40 PRO HG3	4.70	15850.0
HB2	154 LHEM HAP71	4.40	67767.1
HB2	154 LHEM HAP72	5.50 >	14531.3
HB3	40 PRO HG2	3.20	109584.0
HB3	40 PRO HG3	3.30	99843.2
HB3	154 LHEM HAP71	4.10	108328.4
HB3	154 LHEM HAP72	4.50 <	57455.5
HB3	154 LHEM QM8	5.60	16753.4
HG2	154 LHEM HAP71	5.20	26543.7
HG2	154 LHEM HAP72	5.50	17438.3
HG3	154 LHEM HAP71	4.70	44328.2
HG3	154 LHEM HAP72	5.00	33777.0
41 GLY			
QA	42 GLY HN	6.50	1045.0*2
QA	154 LHEM QM5	7.50	3700.4*2
QA	154 LHEM HAP61	6.50	6301.1*2
QA	154 LHEM HAP62	6.50	5260.4*2
42 GLY			
HN	42 GLY HA1	3.30	74740.0
HN	42 GLY HA2	3.40	64060.0
HN	43 GLU- HN	4.90	7166.0
HA1	43 GLU- HN	2.90	165200.0
HA1	43 GLU- HB2	5.00	5820.0
HA1	43 GLU- HB3	5.30	4280.0
HA1	44 GLU- HN	4.40	19120.0
HA1	45 VAL HN	5.50	2977.0
HA2	43 GLU- HN	2.90	150400.0
HA2	43 GLU- HA	4.40	12400.0
HA2	43 GLU- HB3	5.10	5628.0
HA2	44 GLU- HN	4.20	25380.0
HA2	45 VAL HN	5.50	3570.0
43 GLU-			
HN	43 GLU- HA	3.20	87970.0
HN	43 GLU- HB2	3.00	128500.0
HN	43 GLU- HB3	3.20	86960.0
HN	44 GLU- HN	3.10	114300.0
HN	44 GLU- HA	5.30	4362.0
HN	44 GLU- HB2	4.90	6820.0

HN	44 GLU- HB3	5.00	6134.0
HN	45 VAL HN	5.10	8308.0
HA	43 GLU- HB2	3.10	100300.0
HA	43 GLU- HB3	3.30	75960.0
HA	44 GLU- HN	4.00	23430.0
HA	44 GLU- HA	5.10	5603.0
HA	45 VAL HN	5.50	5157.0
HA	45 VAL QG2	6.50	872.0
HA	46 LEU HN	4.30	22100.0
HA	46 LEU HB2	3.80	47830.0
HA	46 LEU QD1	6.00	10950.0
HA	47 ARG+ HN	5.00	9188.0
HA	47 ARG+ QB	6.50	1026.5*2
HA	47 ARG+ QG	6.50	276.5*2
HB2	44 GLU- HN	3.80	34320.0
HB3	44 GLU- HN	4.30	15740.0
44 GLU-			
HN	44 GLU- HA	3.30	78830.0
HN	44 GLU- HB2	3.00	134600.0
HN	44 GLU- HB3	3.20	93960.0
HN	44 GLU- QG	5.60	17095.0*2
HN	45 VAL HN	3.20	91880.0
HN	45 VAL QG1	6.50	4813.0
HN	46 LEU HN	5.00	9714.0
HN	47 ARG+ HN	4.60	15310.0
HN	47 ARG+ QB	6.50	2642.0*2
HA	44 GLU- HB2	3.30	75480.0
HA	44 GLU- HB3	3.40	62720.0
HA	44 GLU- QG	4.80	27110.0*2
HA	45 VAL HN	4.20	17870.0
HA	47 ARG+ HN	4.10	32180.0
HA	47 ARG+ QB	4.70	57200.0*2
HA	47 ARG+ QD	6.50	3539.5*2
HA	48 GLU- HN	4.80	12780.0
HA	48 GLU- HG2	5.00	33920.0
HB2	44 GLU- QG	4.30	91650.0*2
HB2	45 VAL HN	3.80	32210.0
HB2	47 ARG+ QB	6.50	16725.0*2
HB3	44 GLU- QG	4.00	157350.0*2
HB3	45 VAL HN	3.30	75710.0
QG	45 VAL HN	6.50	2395.0*2
QG	47 ARG+ QB	7.50	6930.0*4
QG	47 ARG+ QG	7.50	2173.5*4
45 VAL			
HN	45 VAL HA	3.20	85120.0
HN	45 VAL HB	3.50	48500.0
HN	45 VAL QG1	3.80	82650.0
HN	45 VAL QG2	4.00	63850.0
HN	46 LEU HN	3.40	60060.0
HN	47 ARG+ HN	4.70	14010.0
HN	48 GLU- HN	5.50	1211.0
HA	45 VAL HB	3.10	120600.0
HA	45 VAL QG1	4.40	40830.0
HA	45 VAL QG2	5.00	20990.0
HA	46 LEU HN	4.70	8683.0
HA	48 GLU- HN	4.20	25280.0
HA	48 GLU- HB2	3.70 <	57410.0
HA	48 GLU- HB3	4.50 >	19050.0
HA	48 GLU- HG2	5.00	34190.0
HB	45 VAL QG1	3.80	84720.0
HB	45 VAL QG2	4.00	64650.0
HB	46 LEU HN	4.20	17080.0

HB	154 LHEM QM5	5.10	27700.4
QG1	46 LEU HN	5.50	17210.0
QG1	46 LEU HB3	5.50	17900.0
QG1	154 LHEM QM5	4.30	84851.5
QG2	46 LEU HN	5.20	24450.0
QG2	154 LHEM QM5	4.70	47296.2
46 LEU			
HN	46 LEU HA	4.20	17610.0
HN	46 LEU HB2	3.40 <	60660.0
HN	46 LEU HB3	4.00 >	24130.0
HN	46 LEU QD1	4.90	21580.0
HN	46 LEU QD2	5.00	20290.0
HN	47 ARG+ HN	3.20	92120.0
HN	48 GLU- HN	4.50	19050.0
HA	46 LEU HB2	3.60 >	44410.0
HA	46 LEU HB3	2.70 <	271300.0
HA	46 LEU QD1	3.70 <	87760.0
HA	46 LEU QD2	6.50 >	2782.0
HA	47 ARG+ HN	3.80	30540.0
HA	49 GLN HN	4.80	12340.0
HB2	46 LEU QD1	3.40	246000.0
HB2	46 LEU QD2	3.80	80220.0
HB2	47 ARG+ HN	4.10	21010.0
HB3	46 LEU QD1	6.50	1304.0
HB3	46 LEU QD2	3.40	198400.0
47 ARG+			
HN	47 ARG+ HA	3.60	42870.0
HN	47 ARG+ QB	3.60	123100.0*2
HN	47 ARG+ QG	5.30	22925.0*2
HN	47 ARG+ QD	6.50	3486.0*2
HN	48 GLU- HN	3.20	86920.0
HN	49 GLN HN	5.50	3656.0
HA	47 ARG+ QB	3.60	133800.0*2
HA	47 ARG+ QG	5.20	17015.0*2
HA	47 ARG+ QD	6.30	8700.0*2
HA	48 GLU- HN	3.30	72140.0
HA	49 GLN HN	5.00	9665.0
QB	47 ARG+ QD	5.70	53250.0*4
QB	47 ARG+ HE	5.00	33650.0*2
QB	48 GLU- HN	5.20	17685.0*2
QG	47 ARG+ QD	6.60	17617.5*4
QG	47 ARG+ HE	5.50	20270.0*2
QG	48 GLU- HN	6.10	28445.0*2
QG	50 ALA QB	5.10	101000.0*2
QD	47 ARG+ HE	4.70	54450.0*2
48 GLU-			
HN	48 GLU- HA	3.40	67260.0
HN	48 GLU- HB2	3.00	125100.0
HN	48 GLU- HB3	3.30	71960.0
HN	48 GLU- HG2	3.90 <	41370.0
HN	48 GLU- HG3	4.90 >	12990.0
HN	49 GLN HN	3.30	68790.0
HN	50 ALA HN	4.90	10990.0
HA	48 GLU- HB2	3.70	39200.0
HA	48 GLU- HB3	3.20	92140.0
HA	48 GLU- HG2	3.70	53940.0
HA	48 GLU- HG3	3.80	48130.0
HA	49 GLN HN	3.90	26340.0
HA	50 ALA HN	5.50	1392.0
HB2	48 GLU- HG2	3.20	100100.0
HB3	48 GLU- HG2	4.40	21340.0
HG2	49 GLN HN	5.50	3713.0

HG3	49 GLN HN	5.50	2545.0	QB	57 ASN HN	5.30	4945.0
49 GLN				QB	57 ASN HB2	6.00	10840.0
HN	49 GLN HA	3.30	74650.0	QB	58 PHE HN	4.50	13340.0
HN	49 GLN HB2	3.80	33360.0	QB	154 LHEM QM3	3.60	218939.7
HN	49 GLN HB3	3.60	45060.0	QB	154 LHEM HV4T	5.80	13350.0
HN	49 GLN HG2	4.30	24720.0	QB	154 LHEM HV4C	5.50	17750.0
HN	49 GLN HG3	4.70	15910.0	55 THR			
HN	50 ALA HN	2.90	157900.0	HN	55 THR HA	3.70	38400.0
HN	50 ALA QB	4.70	8075.0	HN	55 THR HB	3.40	62460.0
HN	54 ALA QB	6.50	6823.0	HN	55 THR QG2	5.00	19510.0
HA	49 GLN HB2	3.50	51900.0	HN	56 GLU- HN	4.00	23290.0
HA	49 GLN HB3	3.60	46220.0	HA	55 THR HB	4.00	23460.0
HA	49 GLN HG2	4.10	31100.0	HA	55 THR QG2	3.50	129900.0
HA	49 GLN HG3	4.50	18200.0	HA	56 GLU- HN	4.00	21700.0
HA	50 ALA HN	4.00	23420.0	HA	57 ASN HN	4.90	10180.0
HB2	49 GLN HG2	2.70	242400.0	HA	59 GLU- HN	5.10	8180.0
HB2	49 GLN HG3	2.80	201100.0	HB	55 THR QG2	3.40	205100.0
HB2	50 ALA HN	3.90 >	26120.0	HB	56 GLU- HN	3.00	129000.0
HB2	54 ALA QB	4.00 <	130100.0	HB	59 GLU- HG3	5.40	19730.0
HB3	49 GLN HG2	3.10	134600.0	QG2	56 GLU- HN	4.50	61250.0
HB3	49 GLN HG3	3.50	73300.0	QG2	56 GLU- HA	5.70	15310.0
HB3	50 ALA HN	3.40 <	67210.0	QG2	56 GLU- HB2	6.50	983.0
HB3	54 ALA QB	4.90 >	36040.0	QG2	57 ASN HN	6.30	8068.0
HG2	54 ALA QB	5.20	24220.0	QG2	59 GLU- HN	5.70	15050.0
HG2	57 ASN HB2	4.30	76320.0	QG2	59 GLU- HA	6.50	2714.0
HG3	50 ALA HN	5.50	3048.0	QG2	59 GLU- HB2	5.30	21750.0
50 ALA				QG2	59 GLU- HB3	5.80	13350.0
HN	50 ALA HA	3.40	68290.0	QG2	59 GLU- HG2	4.20	90710.0
HN	50 ALA QB	3.40	215200.0	QG2	59 GLU- HG3	4.40	71570.0
HN	51 GLY HN	4.60	9413.0	56 GLU-			
HA	50 ALA QB	3.40	83090.0	HN	56 GLU- HA	3.30	75680.0
HA	51 GLY HN	2.90	172800.0	HN	56 GLU- HB2	3.70 >	35550.0
QB	51 GLY HN	3.40	55840.0	HN	56 GLU- HB3	3.00 <	125700.0
QB	51 GLY HA1	5.30 <	4845.0	HN	57 ASN HN	3.60	46680.0
QB	51 GLY HA2	6.50 >	1586.0	HA	56 GLU- HB2	3.60	41410.0
51 GLY				HA	56 GLU- HB3	3.30	73310.0
HN	51 GLY HA1	3.20	98420.0	HA	57 ASN HN	4.60	9737.0
HN	51 GLY HA2	3.30	73580.0	HA	57 ASN HA	5.50	3070.0
HN	52 GLY HN	3.70	34640.0	HA	59 GLU- HN	5.00	9681.0
HA1	52 GLY HN	4.10	20560.0	HA	59 GLU- HB2	4.90	10010.0
HA2	52 GLY HN	4.20	16990.0	HA	59 GLU- HB3	4.30	22770.0
52 GLY				HA	59 GLU- HG2	5.50	2965.0
HN	52 GLY HA1	3.70	37670.0	HA	59 GLU- HG3	5.50	6660.0
HN	52 GLY HA2	3.80	33350.0	HA	60 ASP- HN	5.10	8534.0
HN	53 ASP- HN	4.20	18270.0	HB2	57 ASN HN	5.20 >	4864.0
HA1	53 ASP- HN	4.00	23990.0	HB3	57 ASN HN	3.40 <	62240.0
HA1	53 ASP- HA	5.50	1103.0	57 ASN			
HA2	53 ASP- HN	3.90	28160.0	HN	57 ASN HA	3.30	69990.0
HA2	53 ASP- QB	5.90	7000.0*2	HN	57 ASN HB2	3.40	62750.0
53 ASP-				HN	57 ASN HB3	3.20	89950.0
HN	53 ASP- QB	4.70	19660.0*2	HN	58 PHE HN	3.50	50390.0
HA	53 ASP- QB	6.10	476.5*2	HN	59 GLU- HN	5.50	4840.0
QB	55 THR HN	6.50	3560.0*2	HN	60 ASP- HN	5.50	1180.0
54 ALA				HA	57 ASN HB2	3.40	63900.0
HN	54 ALA HA	3.10	104100.0	HA	57 ASN HB3	3.80	31670.0
HN	54 ALA QB	3.40	77710.0	HA	59 GLU- HN	5.00	9395.0
HN	55 THR HN	3.20	99370.0	HA	60 ASP- HN	4.00	37720.0
HN	55 THR HB	5.50	3369.0	HA	60 ASP- HB2	4.00	35650.0
HA	54 ALA QB	4.30	13180.0	HA	60 ASP- HB3	4.10	32580.0
HA	55 THR HN	4.00	22170.0	HB2	58 PHE HN	4.50 >	10990.0
QB	55 THR HN	4.40	12030.0	HB2	154 LHEM HV4T	4.70	45680.0
QB	55 THR HA	5.00	6379.0	HB2	154 LHEM HV4C	4.60	56880.0

HB3	58 PHE HN	3.50 <	54150.0
HB3	154 LHEM HV4T	5.00	31480.0
58 PHE			
HN	58 PHE HB2	3.40	68480.0
HN	59 GLU- HN	3.50	56160.0
HN	154 LHEM QM3	5.40	19607.2
HB2	59 GLU- HN	3.70	40220.0
59 GLU-			
HN	59 GLU- HA	3.60	40870.0
HN	59 GLU- HB2	3.80	31960.0
HN	59 GLU- HB3	3.70	36200.0
HN	59 GLU- HG2	4.10	30800.0
HN	59 GLU- HG3	4.40	21400.0
HN	60 ASP- HN	3.10	114600.0
HN	60 ASP- HB3	3.80	30950.0
HA	59 GLU- HB2	3.20	89050.0
HA	59 GLU- HB3	3.30	74170.0
HA	59 GLU- HG2	3.90	37950.0
HA	59 GLU- HG3	3.90	42140.0
HA	60 ASP- HN	4.00	23890.0
HA	60 ASP- HA	5.50	3160.0
HA	61 VAL HN	5.50	5570.0
HA	62 GLY HN	4.10	32240.0
HA	62 GLY HA1	5.50	3213.0
HA	62 GLY HA2	5.50	1910.0
HA	63 HIS HN	5.50	1884.0
HB2	59 GLU- HG2	3.10	119000.0
HB2	59 GLU- HG3	3.70	51000.0
HB2	60 ASP- HN	3.70	38060.0
HB3	59 GLU- HG2	3.40	83710.0
HB3	59 GLU- HG3	3.10	132000.0
HB3	60 ASP- HN	3.30	71350.0
60 ASP-			
HN	60 ASP- HA	3.10	102900.0
HN	60 ASP- HB2	2.80 <	216900.0
HN	60 ASP- HB3	3.30 >	71460.0
HN	61 VAL HN	3.20	84620.0
HA	60 ASP- HB2	3.20	97330.0
HA	60 ASP- HB3	3.20	95840.0
HB2	61 VAL HN	4.20	17800.0
HB3	61 VAL HN	3.90	26180.0
61 VAL			
HN	61 VAL HA	3.30	75880.0
HN	61 VAL HB	3.90	29180.0
HN	61 VAL QQG	8.20	4404.0*2
HN	62 GLY HN	3.30	71840.0
HN	62 GLY HA1	5.50	1048.0
HN	63 HIS HN	5.50	4470.0
HA	61 VAL HB	3.40	67270.0
HA	61 VAL QQG	4.40	80300.0*2
HB	61 VAL QQG	6.20	25180.0*2
62 GLY			
HN	62 GLY HA1	3.00	132000.0
HN	62 GLY HA2	3.50	56820.0
HN	63 HIS HN	3.80	29570.0
HA1	63 HIS HN	4.60	10360.0
HA2	63 HIS HN	4.40	13170.0
63 HIS			
HN	63 HIS HA	4.80	7606.0
HN	63 HIS HB2	5.50 >	1744.0
HN	63 HIS HB3	4.20 <	16330.0
HN	64 SER HN	4.80	7830.7

HA	63 HIS HB2	5.50 >	1648.0
HA	63 HIS HB3	5.20 <	4654.0
HA	64 SER HN	2.70	274683.0
HB2	64 SER HN	4.00 <	23747.0
HB3	64 SER HN	4.70 >	8371.0
64 SER			
HN	64 SER HA	3.50	55667.2
HN	64 SER HB2	3.70	36052.4
HN	64 SER HB3	3.20	84775.4
HN	65 THR HN	4.60	9428.8
HN	66 ASP- HN	5.50	2514.0
HN	67 ALA HN	4.90	10908.9
HN	68 ARG+ HN	5.50	2343.9
HA	64 SER HB2	5.20 >	4636.0
HA	64 SER HB3	3.90 <	26610.0
HA	65 THR HN	2.80	196000.0
HA	65 THR HB	5.50	3102.0
HA	67 ALA HN	5.20	7238.0
HA	68 ARG+ QG	6.50	1225.5*2
HB2	65 THR HN	3.10	115100.0
HB3	65 THR HN	3.60	47110.0
HB3	67 ALA HN	5.50	5571.0
65 THR			
HN	65 THR HA	4.10	19820.0
HN	65 THR HB	3.50	51240.0
HN	66 ASP- HN	3.40	61770.0
HN	67 ALA HN	5.00	9918.0
HA	65 THR HB	5.00	6178.0
HA	66 ASP- HN	3.60	42530.0
HA	68 ARG+ HN	5.30	6408.0
HA	68 ARG+ HB2	4.80 <	12510.0
HA	68 ARG+ HB3	5.50 >	3957.0
HA	68 ARG+ QD	6.50	2269.0*2
HB	66 ASP- HN	4.10	19670.0
66 ASP-			
HN	66 ASP- HA	3.00	146800.0
HN	66 ASP- HB2	3.30 <	82430.0
HN	66 ASP- HB3	4.00 >	22980.0
HN	67 ALA HN	3.60	47790.0
HN	68 ARG+ HN	5.50	5015.0
HA	66 ASP- HB2	3.00	146300.0
HA	66 ASP- HB3	3.30	78130.0
HA	67 ALA HN	3.80	32770.0
HA	69 GLU- HN	4.50	17670.0
HA	69 GLU- QB	6.00	9700.0*2
HA	70 LEU HN	4.80	12180.0
HB2	67 ALA HN	3.20	84540.0
HB3	67 ALA HN	3.50	49170.0
67 ALA			
HN	67 ALA HA	3.60	43100.0
HN	67 ALA QB	5.70	3161.0
HN	68 ARG+ HN	3.30	69630.0
HN	69 GLU- HN	4.60	15630.0
HN	70 LEU HN	5.10	8439.0
HN	70 LEU HB2	5.50	1170.0
HN	70 LEU HB3	5.50	725.0
HA	67 ALA QB	3.60	32580.0
HA	70 LEU HN	5.10	8787.0
HA	70 LEU HB2	5.10 >	8686.0
HA	70 LEU HB3	4.00 <	37710.0
QB	68 ARG+ QG	7.50	2825.0*2
68 ARG+			

HN	68 ARG+ HA	3.60	47680.0	HA	73 THR HB	5.50	2489.0
HN	68 ARG+ HB2	3.80 >	33580.0	HA	74 TYR CZ	7.50	5450.0*2
HN	68 ARG+ HB3	3.20 <	95610.0	HB2	70 LEU QD1	3.60	104600.0
HN	68 ARG+ QG	4.80	42655.0*2	HB2	71 SER HN	3.90	25710.0
HN	68 ARG+ QD	5.00	34260.0*2	HB2	74 TYR CZ	7.50 >	1061.0*2
HN	69 GLU- HN	3.20	97940.0	HB3	70 LEU HG	3.20	103700.0
HN	70 LEU HN	4.90	10320.0	HB3	70 LEU QD1	3.60	109600.0
HN	71 SER HN	5.50	2341.0	HB3	70 LEU QD2	4.20	50130.0
HA	68 ARG+ HB2	3.40	57670.0	HB3	74 TYR CZ	7.50 <	9240.0*2
HA	68 ARG+ HB3	3.40	64620.0	HG	70 LEU QD1	3.40	181800.0
HA	68 ARG+ QG	4.60	34445.0*2	HG	70 LEU QD2	3.40	165100.0
HA	68 ARG+ QD	5.40	22315.0*2	HG	74 TYR CZ	6.70	48785.0*2
HA	69 GLU- HN	4.60	9582.0	QD1	73 THR HB	5.70	14840.0
HA	71 SER HN	4.50	18530.0	QD1	74 TYR CG	8.50 >	3452.5*2
HA	71 SER QB	6.30	6960.0*2	QD1	74 TYR CZ	7.30	23390.0*2
HA	72 LYS+ HN	5.20	7097.0	QD2	73 THR HB	5.90	11450.0
HB2	68 ARG+ QD	4.20	100650.0*2	QD2	74 TYR CG	8.10 <	9470.0*2
HB2	69 GLU- HN	4.50 >	10700.0	QD2	74 TYR CZ	7.40	20290.0*2
HB2	69 GLU- HA	4.80	7664.0	71 SER			
HB3	68 ARG+ QD	4.40	75200.0*2	HN	71 SER HA	3.10	106800.0
HB3	69 GLU- HN	3.60 <	45420.0	HN	71 SER QB	5.30	8640.0*2
HB3	69 GLU- HA	5.10	5505.0	HN	72 LYS+ HN	3.80	30670.0
QG	68 ARG+ QD	6.30	24857.5*4	HN	74 TYR CG	6.50	62650.0*2
QG	69 GLU- HN	5.90	36975.0*2	HN	74 TYR CZ	7.50	3657.5*2
QG	69 GLU- HA	6.50	2386.0*2	HA	71 SER QB	4.00	148250.0*2
69 GLU-				HA	72 LYS+ HN	3.60	44130.0
HN	69 GLU- HA	3.30	77570.0	HA	72 LYS+ HA	5.50	1905.0
HN	69 GLU- QB	4.20	46800.0*2	HA	74 TYR HN	4.80	12160.0
HN	69 GLU- HG2	4.20 >	28820.0	HA	74 TYR HB2	5.30	6466.0
HN	69 GLU- HG3	3.20 <	107900.0	HA	74 TYR CG	6.10	115500.0*2
HN	70 LEU HN	3.10	109900.0	HA	74 TYR CZ	7.20	24340.0*2
HN	70 LEU HB3	5.50	555.0	QB	72 LYS+ HN	5.40	12760.0*2
HN	71 SER HN	5.30	6364.0	QB	74 TYR CG	8.20	24277.5*4
HN	72 LYS+ HN	5.50	912.0	QB	74 TYR CZ	8.50	3715.0*4
HA	69 GLU- QB	4.60	45745.0*2	72 LYS+			
HA	69 GLU- HG2	4.30 >	23570.0	HN	72 LYS+ HA	3.40	61960.0
HA	69 GLU- HG3	3.50 <	65960.0	HN	72 LYS+ HB2	3.00	125000.0
HA	70 LEU HN	4.20	17430.0	HN	72 LYS+ HB3	3.30	80730.0
HA	72 LYS+ HN	4.60	14830.0	HN	73 THR HN	3.30	70360.0
HA	72 LYS+ HB2	4.70	14150.0	HN	73 THR HA	5.50	1579.0
QB	69 GLU- HG2	4.50 >	67400.0*2	HN	74 TYR CG	6.60	54950.0*2
QB	69 GLU- HG3	3.70 <	243400.0*2	HA	72 LYS+ HB2	3.20 <	93610.0
QB	70 LEU HN	5.20	18130.0*2	HA	72 LYS+ HB3	3.80 >	29780.0
HG2	70 LEU HN	5.40	20880.0	HA	73 THR HN	4.10	19860.0
HG3	70 LEU HN	4.70	44980.0	HA	74 TYR HN	4.80	12140.0
70 LEU				HA	75 ILE HN	4.10	30190.0
HN	70 LEU HA	3.50	51060.0	HA	75 ILE HB	4.50	17670.0
HN	70 LEU HB2	3.10	111400.0	HA	75 ILE QG2	4.20	86960.0
HN	70 LEU HB3	2.90	170000.0	HA	75 ILE HG13	5.50	17950.0
HN	70 LEU HG	5.10	9783.0	HA	75 ILE QD1	6.50	5081.0
HN	70 LEU QD1	5.10	17810.0	HB2	73 THR HN	3.10	110600.0
HN	70 LEU QD2	5.70	10370.0	HB2	74 TYR HN	4.30	24260.0
HN	71 SER HN	3.30	77740.0	HB3	73 THR HN	3.30	71490.0
HN	72 LYS+ HN	4.60	14670.0	73 THR			
HA	70 LEU HB2	3.30 <	78920.0	HN	73 THR HA	3.30	77800.0
HA	70 LEU HB3	4.10 >	20400.0	HN	73 THR HB	3.20	88730.0
HA	70 LEU HG	3.80	45660.0	HN	73 THR QG2	4.30	41500.0
HA	70 LEU QD1	4.30 <	43400.0	HN	74 TYR HN	3.00	148100.0
HA	70 LEU QD2	6.20 >	7104.0	HN	74 TYR CG	7.50	13120.0*2
HA	71 SER HN	4.40	13540.0	HN	74 TYR CZ	7.50	1623.5*2
HA	72 LYS+ HN	4.70	13580.0	HN	75 ILE HN	4.60	14900.0
HA	73 THR HN	3.90	41170.0	HA	73 THR QG2	3.60	102800.0

HA	74 TYR HN	4.50	12030.0
HA	74 TYR CZ	7.50	1171.0*2
HA	75 ILE HN	5.50	4203.0
HB	73 THR QG2	3.40	143300.0
HB	74 TYR HN	3.60	43290.0
HB	75 ILE HN	5.50	4011.0
QG2	74 TYR HN	4.50	62680.0
QG2	74 TYR CZ	8.00	10610.0*2
74 TYR			
HN	74 TYR HA	3.70	36880.0
HN	74 TYR HB2	3.50	57400.0
HN	74 TYR HB3	3.90	28730.0
HN	74 TYR CG	4.80	226100.0*2
HN	75 ILE HN	2.80	200100.0
HN	75 ILE HB	3.80	32980.0
HA	74 TYR HB2	3.20	99750.0
HA	74 TYR HB3	3.20	83920.0
HA	74 TYR CG	4.50	71050.0*2
HA	74 TYR CZ	6.10	6015.0*2
HA	75 ILE HN	4.10	21220.0
HB2	74 TYR CG	5.40	74900.0*2
HB2	74 TYR CZ	7.30	8765.0*2
HB2	75 ILE HN	3.90	27300.0
HB2	75 ILE HA	5.50	1830.0
HB3	74 TYR CG	5.50	67500.0*2
HB3	74 TYR CZ	7.30	8075.0*2
HB3	75 ILE HN	4.20	16210.0
CG	74 TYR CZ	7.30	99300.0*4
75 ILE			
HN	75 ILE HA	3.70	40160.0
HN	75 ILE HB	2.80	197600.0
HN	75 ILE QG2	4.50	35270.0
HN	75 ILE HG12	4.60	17270.0
HN	75 ILE HG13	4.70	15240.0
HN	75 ILE QD1	6.00	8385.0
HN	76 ILE HN	4.70	8303.0
HA	75 ILE HB	4.00	24960.0
HA	75 ILE QG2	5.60	11170.0
HA	75 ILE HG12	4.60 >	16650.0
HA	75 ILE HG13	3.70 <	53100.0
HA	75 ILE QD1	4.30	43400.0
HA	76 ILE HN	3.10	119200.0
HA	76 ILE QG2	5.70	14090.0
HA	76 ILE HG12	5.50	10820.0
HA	76 ILE HG13	5.50	7603.0
HA	76 ILE QD1	6.50	3423.0
HA	77 GLY HN	4.10	29600.0
HB	75 ILE QG2	3.50	126800.0
HB	75 ILE HG12	2.90	185800.0
HB	75 ILE HG13	3.10	121400.0
HB	75 ILE QD1	4.30	45360.0
QG2	75 ILE HG12	3.60	114700.0
QG2	75 ILE HG13	3.90	75990.0
QG2	75 ILE QD1	4.50	125100.0
QG2	76 ILE HN	6.00	11090.0
QG2	77 GLY HN	6.50	3337.0
HG12	75 ILE QD1	3.40 <	218700.0
HG12	77 GLY HN	4.90 >	35590.0
HG13	75 ILE QD1	4.10 >	56890.0
HG13	76 ILE HN	4.50	61030.0
HG13	77 GLY HN	4.00 <	130200.0
QD1	76 ILE HN	6.50	2821.0

QD1	77 GLY HN	6.50	4903.0
76 ILE			
HN	76 ILE HA	3.50	49320.0
HN	76 ILE HB	5.00	5977.0
HN	76 ILE QG2	5.00	20820.0
HN	76 ILE HG12	4.10	30690.0
HN	76 ILE HG13	3.90	39790.0
HN	76 ILE QD1	5.30	14920.0
HN	77 GLY HN	3.20	88510.0
HA	76 ILE HB	3.70	36320.0
HA	76 ILE QG2	3.40	152200.0
HA	76 ILE HG12	4.80	13920.0
HA	76 ILE HG13	5.50	6287.0
HA	76 ILE QD1	5.80	10010.0
HA	77 GLY HN	4.30	15020.0
HB	76 ILE QG2	3.40	174000.0
HB	76 ILE HG12	3.80	45150.0
HB	76 ILE HG13	4.10	32720.0
HB	76 ILE QD1	3.40	185700.0
QG2	76 ILE HG12	4.40	40060.0
QG2	76 ILE HG13	4.00	66800.0
QG2	76 ILE QD1	4.70	97220.0
QG2	77 GLY HN	6.50	6328.0
HG12	76 ILE QD1	3.60	105600.0
HG12	77 GLY HN	5.50	14650.0
HG13	76 ILE QD1	3.70	88510.0
HG13	77 GLY HN	5.50	15270.0
QD1	77 GLY HN	6.50	6864.0
QD1	77 GLY HA2	6.50	3614.0
77 GLY			
HN	77 GLY HA1	3.80	33300.0
HN	77 GLY HA2	3.50	55480.0
HN	78 GLU- HN	4.90	7239.0
HA1	78 GLU- HN	3.40	61080.0
HA2	78 GLU- HN	3.40	60880.0
78 GLU-			
HN	78 GLU- HA	4.00	22830.0
HN	78 GLU- QB	5.00	13800.0*2
HN	78 GLU- QG	5.80	13480.0*2
HA	78 GLU- QB	5.70	8555.0*2
HA	78 GLU- QG	4.40	44520.0*2
HA	79 LEU HN	5.50	1197.0
QB	78 GLU- QG	5.80	43975.0*4
79 LEU			
HN	79 LEU HA	4.70	8575.0
HN	79 LEU QB	4.90	14065.0*2
HN	79 LEU HG	4.30	24270.0
HN	79 LEU QD1	4.50	34220.0
80 HIS			
HN	80 HIS HA	4.30	15060.0
HN	80 HIS HB2	3.40	65950.0
HN	80 HIS HB3	3.10	107800.0
HN	80 HIS HD2	4.80	14550.0
HA	80 HIS HB2	4.10	20340.0
HA	80 HIS HB3	3.60	45100.0
HA	80 HIS HD2	4.30	23340.0
HA	81 PRO HG2	5.50 >	11640.0
HA	81 PRO HG3	4.50 <	61760.0
HA	81 PRO QD	6.00	32240.0*2
HA	82 ASP- HN	5.50	2658.0
HB2	80 HIS HD2	4.00	35900.0
HB2	82 ASP- HN	5.00	9161.0

HB3	80 HIS	HD2	4.00	32850.0
HB3	81 PRO	QD	6.50	13290.0*2
HB3	82 ASP-	HN	4.90	10860.0
HD2	80 HIS	HE1	4.50	19720.0
HD2	81 PRO	QD	6.50	3571.0*2
HD2	82 ASP-	HN	5.50	1707.0
HE1	82 ASP-	HN	4.70	45660.0
HE1	82 ASP-	HA	5.50	3397.0
HE1	82 ASP-	HB2	4.90	34500.0
HE1	82 ASP-	HB3	4.90	35130.0
81 PRO				
HA	81 PRO	HB2	3.10	119200.0
HA	81 PRO	HB3	3.40	64920.0
HA	81 PRO	HG2	3.90	37320.0
HA	81 PRO	HG3	3.80	44240.0
HA	82 ASP-	HN	5.20	4697.0
HA	84 ARG+	HN	4.50	17650.0
HA	84 ARG+	HB2	5.40 >	5815.0
HA	84 ARG+	HB3	4.50 <	17110.0
HB2	81 PRO	HG2	2.70	277400.0
HB2	81 PRO	HG3	3.70	53650.0
HB2	82 ASP-	HN	4.90 >	6656.0
HB3	81 PRO	QD	5.90	12610.0*2
HB3	82 ASP-	HN	4.10 <	19470.0
HG2	81 PRO	QD	4.30	92700.0*2
HG2	82 ASP-	HN	5.50 >	1419.0
HG3	81 PRO	QD	4.70	49490.0*2
HG3	82 ASP-	HN	5.50 <	17740.0
QD	82 ASP-	HN	6.50	1501.0*2
82 ASP-				
HN	82 ASP-	HA	3.80	32510.0
HN	82 ASP-	HB2	3.30	77210.0
HN	82 ASP-	HB3	3.60	43920.0
HN	83 ASP-	HN	3.30	70790.0
HN	84 ARG+	HN	5.50	4039.0
HA	82 ASP-	HB2	3.70	40420.0
HA	82 ASP-	HB3	3.60	45760.0
HA	83 ASP-	HN	4.10	20150.0
HA	85 SER	HN	5.50	5556.0
HB3	83 ASP-	HN	4.20	18410.0
83 ASP-				
HN	83 ASP-	HA	3.30	77490.0
HN	83 ASP-	HB2	2.90 <	168900.0
HN	83 ASP-	HB3	3.40 >	59800.0
HN	84 ARG+	HN	3.10	110400.0
HN	85 SER	HN	5.50	3737.0
HA	83 ASP-	HB2	3.60	43060.0
HA	83 ASP-	HB3	3.30	82240.0
HA	84 ARG+	HN	4.30	15010.0
HA	86 LYS+	HN	5.40	6065.0
HA	86 LYS+	HB2	4.60 <	16590.0
HA	86 LYS+	HB3	5.50 >	1029.0
84 ARG+				
HN	84 ARG+	HA	3.80	31220.0
HN	84 ARG+	HB2	4.50 >	11410.0
HN	84 ARG+	HB3	2.80 <	213600.0
HN	85 SER	HN	4.20	18450.0
HN	86 LYS+	HN	4.60	15520.0
HA	84 ARG+	HB2	4.00	23280.0
HA	84 ARG+	HB3	4.10	20590.0
HA	87 ILE	HN	5.20	7623.0
HA	87 ILE	HB	5.50	4751.0
85 SER				
HN	85 SER	HA	3.50	48320.0
HN	86 LYS+	HN	3.80	31440.0
HN	87 ILE	HN	5.30	6384.0
86 LYS+				
HN	86 LYS+	HA	4.00	24090.0
HN	86 LYS+	HB2	5.50 >	1286.0
HN	86 LYS+	HB3	3.20 <	88760.0
HN	86 LYS+	QG	6.50	6770.0*2
HN	87 ILE	HN	4.00	24290.0
HA	86 LYS+	HB2	3.30	68990.0
HA	86 LYS+	HB3	3.30	77930.0
HA	86 LYS+	QG	6.00	7915.0*2
HA	87 ILE	HN	4.50	12060.0
HB2	86 LYS+	QG	5.40 >	21900.0*2
HB3	86 LYS+	QG	4.60 <	60300.0*2
87 ILE				
HN	87 ILE	HA	4.20	16650.0
HN	87 ILE	HB	3.20	90670.0
HN	87 ILE	HG12	3.80	44220.0
HN	87 ILE	HG13	3.80	48130.0
HN	87 ILE	QD1	4.70	28740.0
HA	87 ILE	HB	3.10	107000.0
HA	87 ILE	HG12	5.20 >	8976.0
HA	87 ILE	HG13	3.40 <	83880.0
HA	88 ALA	HN	3.60	43800.0
HB	87 ILE	HG12	4.20 >	28860.0
HB	87 ILE	HG13	3.00 <	156600.0
88 ALA				
HN	88 ALA	HA	3.10	105000.0
HN	88 ALA	QB	3.40	87390.0
HN	89 LYS+	HN	4.80	7638.0
HA	88 ALA	QB	3.40	123800.0
HA	89 LYS+	HN	3.50	51760.0
QB	89 LYS+	HN	3.90	22030.0
89 LYS+				
HN	89 LYS+	HA	4.10	19350.0
91 SER				
HN	91 SER	HA	4.30	14940.0
HN	91 SER	QB	5.70	5305.0*2
HA	91 SER	QB	6.50	241.5*2
92 GLU-				
HN	92 GLU-	HA	5.50	.0
HN	92 GLU-	QG	4.30	92950.0*2
154 LHEM				
HAP71	154 LHEM	HAP72	2.40	430726.0
HAP71	154 LHEM	HBP73	2.90	176095.4
HAP71	154 LHEM	HBP74	2.70	253603.2
HAP71	154 LHEM	QM8	4.60	31631.0
HAP71	154 LHEM	HGM	3.30	86107.1
HAP71	154 LHEM	HAP61	5.50	1925.3
HAP71	154 LHEM	HAP62	5.20	9695.1
HAP72	154 LHEM	HBP73	3.10	126744.6
HAP72	154 LHEM	QM8	3.90	71690.0
HBP73	154 LHEM	QM8	5.50	12465.2
HBP73	154 LHEM	HGM	3.50	64152.3
HBP73	154 LHEM	HAP61	5.50	4916.1
HBP73	154 LHEM	HAP62	5.20	9177.7
HBP73	64 SER	HN	5.50	5041.6
HBP74	64 SER	HN	5.50	6050.0
QM8	67 ALA	HA	5.80	12990.0
QM1	154 LHEM	HV2A	4.30	43909.7

QM1	154 LHEM HV2T	5.60	11224.8
QM1	154 LHEM HV2C	4.10	56428.2
QM1	67 ALA HA	6.00	10970.0
QM1	70 LEU HN	5.80	13520.0
QM1	70 LEU HB2	5.50	18320.0
QM1	70 LEU HB3	5.10	27640.0
QM1	70 LEU HG	5.00	30790.0
QM1	70 LEU QD1	4.30	80380.0
QM1	71 SER HN	4.70	46010.0
QM1	71 SER HA	4.10	107100.0
QM1	71 SER QB	6.70	15220.0*2
QM1	74 TYR CG	7.20	25635.0*2
QM1	74 TYR CZ	7.50	18475.0*2
HV2A	154 LHEM HV2T	3.60	56390.1
HV2A	154 LHEM HV2C	3.80	42654.1
HV2A	154 LHEM HAM	3.70	54031.0
HV2A	154 LHEM QM3	5.50	12294.0
HV2A	71 SER HA	5.00	33982.5
HV2A	71 SER QB	6.50	10385.7*2
HV2A	74 TYR CG	7.50	9691.3*2
HV2A	74 TYR CZ	7.50	443.3*2
HV2T	154 LHEM HAM	5.10	9824.5
HV2T	71 SER HN	5.50	6403.8
HV2T	71 SER HA	4.60	50606.5
HV2T	71 SER QB	6.00	31885.9*2
HV2T	74 TYR HB2	5.50	9523.9
HV2T	74 TYR CG	7.50	11169.6*2
HV2C	154 LHEM HAM	4.00	34549.4
HV2C	71 SER HN	5.50	11357.9
HV2C	71 SER HA	4.70	45165.4
HV2C	71 SER QB	6.50	11886.8*2
HV2C	74 TYR HB2	5.50	3135.3
HV2C	74 TYR CG	7.50	16622.1*2
HAM	154 LHEM QM3	3.50	131500.8
QM3	154 LHEM HV4A	5.20	16411.0
QM3	154 LHEM HV4T	4.60	32704.0
QM3	154 LHEM HV4C	3.50	121151.2
QM3	63 HIS HE1	5.00	15590.0
HV4A	154 LHEM HV4T	4.70	15590.0
HBM	154 LHEM QM5	4.10	54183.2
QM5	154 LHEM HAP61	4.10	57759.9
QM5	154 LHEM HAP62	4.90	22240.2
QM5	154 LHEM HBP63	4.30	43833.6
QM5	154 LHEM HBP64	4.80	24146.5
HGM	154 LHEM HAP61	4.20	27491.1
HGM	154 LHEM HAP62	3.70	50226.0
HAP61	154 LHEM HAP62	3.50	71001.3
HAP61	154 LHEM HBP63	2.90	172252.4
HAP61	154 LHEM HBP64	3.50	67462.6
HAP62	154 LHEM HBP63	3.40	75491.2
HAP62	154 LHEM HBP64	3.30	96228.5
HBP63	154 LHEM HBP64	2.80	195700.0

Stereospecific assignment for diastereotopic pairs of methylene protons or isopropyl methyl groups

H α 1/H α 2	42
H β 1/H β 2	6 7 15 20 22 25 30 31 34 36 44 48 49 70 74 83
H γ 1/H γ 2	48 81
7-H α 1/H α 2	63
7-H β 1/H β 2	63
δ -CH ₃	9 25 32 36
γ -CH ₃	23 29