SUPPORTING INFORMATION

Solution structure and characterization of the heme chaperone CcmE

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- ¹H, ¹⁵N and ¹³C Chemical Shifts
- Angle constraints
- Experimentally determined hydrogen bonds
- Experimental upper distance limits and NOE intensities

^1H , ^{15}N and ^{13}C resonance assignments for the apoCcmE at 298 K, pH 7.0, in water solution.

Residue	N (NH) ppm	C α (H α) ppm	CO ppm	C β (H β) Ppm	Other ppm
L-30	123.02 (8.38)	53.29 (3.62)	175.04	39.68	
N-31	118.16 (8.41)	51.11 (4.61)	173.3	36.36	
S-32	115.57 (8.07)	56.59 (4.27)	172.1	61.31	
N-33	119.46 (8.38)	50.98 (4.20)	172.88	36.12	
L-34	120.75 (7.93)	53.08 (4.10)	174.64	39.96	
N-35	118.49 (8.26)	50.79 (4.59)	172.32	36.02	
L-36	121.40 (8.10)	53.12 (4.15)	172.61	40.38 (1.60, 1.35)	C γ 24.60 (1.50), C δ 1 22.6 (0.82), C δ 2 20.90 (0.75)
F-37	119.78 (7.77)	54.46 (4.89)	172.61	38.76 (2.82, 2.72)	H ζ (6.77), H γ (6.87); H ζ (7.06)
Y-38	125.29 (8.64)	54.98 (4.60)	172.82	40.49 (2.93, 2.37)	H γ (6.90), H ζ (6.99)
T-39	110.16 (8.45)	57.39 (5.03)		65.71 (4.88)	C γ 19.89 (1.38)
P-40		64.06 (3.82)	176.17	29.49 (1.97)	C γ 26.51 (1.32, 1.65), C δ 47.00 (4.16, 3.94)
S-41	112.01 (8.95)	61.13 (3.97)	173.60	59.88 (3.69, 3.80)	
E-42	120.10 (7.64)	55.14 (3.95)	176.38	29.96 (2.61, 1.86)	C γ 35.60 (2.48, 2.24)
I-43	118.81 (7.51)	62.02 (3.15)	173.93	34.31 (1.96)	C γ 1 26.20 (1.49, 0.60), C γ 2 14.80 (0.59), C δ 11.30 (0.41)
V-44	112.66 (6.84)	61.95 (3.77)	175.03	30.39 (1.90)	C γ 1 18.90 (0.93), C γ 2 18.70 (0.86)
N-45	113.63 (8.15)	51.46 (4.76)	174.00	38.12 (2.78, 2.69)	N δ 113.63 (7.36, 6.95)
G-46	109.74 (7.77)	41.72 (3.88, 3.48)	170.59		
K-47	119.13 (7.97)	53.73 (4.12)	176.70	29.75 (2.06, 1.80)	C γ 22.20 (1.50), C δ 25.50 (1.34, 1.28), C ϵ 39.08 (2.83, 2.59)
T-48	120.10 (9.37)	63.46 (3.81)	172.98	66.55 (4.12)	C γ 19.30 (1.19)
D-49	116.87 (8.73)	53.41 (4.41)	175.36	37.37 (2.68)	
T-50	107.47 (7.64)	59.36 (4.32)	174.01	68.42 (4.27)	C γ 19.00 (1.09)
G-51	110.71 (8.40)	43.41 (4.06, 3.75)	171.66		
V-52	119.46 (7.40)	61.25 (3.89)	174.08	30.43 (1.80)	C γ 19.00 (0.85, 0.82)
K-53	129.17 (8.66)	51.51 (4.62)		31.02 (1.71, 1.54)	C γ 22.25 (1.60, 1.33), C δ 26.79 (1.56), C ϵ (2.84, 2.70)
P-54		59.78 (4.47)	172.58	29.38 (1.67, 1.44)	C γ 24.67 (1.42, 0.80), C δ 47.05 (3.59, 3.25)
E-55	118.16 (7.68)	51.64 (4.30)	173.14	30.17 (1.94, 1.63)	C γ 33.60 (2.14)
A-56	122.37 (8.39)	50.86 (3.72)	174.46	15.41 (1.15)	
G-57	110.71 (9.26)	42.52 (4.21, 3.37)	171.84		
Q-58	120.10 (7.79)	53.53 (4.20)	172.54	27.61 (2.11, 1.86)	C γ 32.00 (2.36, 2.28), N ϵ 111.36 (7.61, 6.90)
R-59	123.69 (8.36)	53.18 (4.85)	173.69	27.77 (1.71, 1.60)	C γ 25.4 (1.52, 1.34), C δ 41.16 (3.06)
I-60	119.13 (8.82)	57.30 (4.92)	171.15	40.91 (1.94)	C γ 1 22.5 (0.99, 0.77), C γ 2 15.90 (0.73), C δ 12.55 (0.34)
R-61	119.46 (8.41)	51.95 (5.27)	172.10	31.44 (1.62, 1.58)	C γ 26.10 (1.50, 1.39), C δ 42.90 (3.11)
V-62	120.43 (9.02)	56.36 (5.20)	171.36	32.90 (1.49)	C γ 1 20.10 (0.60), C γ 2 17.90 (0.52)
G-63	112.01 (7.27)	41.34 (5.20, 3.20)	169.49		
G-64	105.21 (7.75)	42.83 (3.70, 3.58)	168.30		
M-65	117.84 (8.61)	50.72 (4.56)	173.45	31.27 (1.05, 0.84)	C γ 39.30 (2.22, 2.16), C ϵ 30.98 (1.94)
V-66	122.70 (8.08)	60.74 (4.41)	175.43	29.54 (1.91)	C γ 1 20.40 (0.53), C γ 2 18.60 (0.83)
T-67	127.88 (9.13)	61.37 (4.20)	173.29	66.59 (3.95)	C γ 19.30 (1.24)
V-68	133.06 (9.39)	62.26 (3.76)	174.80	28.96 (1.93)	C γ 1 19.50 (0.95), C γ 2 18.20 (0.87)
G-69	116.54 (9.38)	43.26 (4.08, 3.84)	172.73		
S-70	112.66 (7.70)	56.79 (4.34)	171.86	63.00 (4.07, 3.49)	H η (6.12)
M-71	122.70 (8.37)	54.28 (5.09)	174.47	30.22 (2.08, 2.00)	C γ 29.80 (2.38, 2.34), C ϵ 26.40 (1.76)
V-72	128.53 (9.43)	59.73 (4.22)	172.89	32.05 (1.93)	C γ 18.30 (0.86, 0.83)
R-73	126.91 (8.74)	52.18 (4.75)	172.97	29.77 (1.77, 1.54)	C γ 25.40 (1.46), C δ 40.93 (3.06)
D-74	125.94 (8.43)	49.14 (4.83)		40.47 (2.90, 2.60)	
P-75		61.66 (4.31)	174.81	29.87 (2.24, 1.81)	C γ 24.60 (1.94, 1.90), C δ 48.60 (3.87, 3.84)
N-76	113.63 (8.25)	50.83 (4.75)	172.00	37.57 (2.87, 2.63)	N δ 114.28 (7.73, 6.88)
S-77	114.60 (7.77)	55.76 (4.54)	170.58	62.87 (3.94, 3.70)	

L-78	117.84 (8.16)	52.47 (1.42, 1.31)	173.86	38.94 (1.42, 1.31)	C γ 24.30 (1.47), C δ 1 23.10 (0.76), C δ 2 20.40 (0.68)
H-79	117.19 (8.16)	55.28 (4.75)	172.65	26.84 (3.03, 2.97)	Ne1 178.30 (8.08), Ne2 187.55, H δ 2 (7.08)
V-80	123.67 (8.78)	56.77 (5.04)	170.05	33.71 (2.08)	C γ 19.00 (0.97, 0.94)
Q-81	121.40 (8.16)	50.97 (5.45)	171.00	31.78 (2.19, 1.94)	C γ 32.60 (1.88, 1.79), Ne 113.62 (7.85, 6.94)
F-82	118.49 (8.59)	53.53 (4.98)	168.70	37.21 (3.25, 3.00)	Cz (6.90), Cg (6.84), Hz (6.49)
A-83	118.81 (8.74)	47.56 (5.48)	174.39	19.06 (1.25)	
V-84	117.51 (8.82)	57.34 (5.00)	172.10	32.50 (1.52)	C γ 1 20.10 (0.72), C γ 2 18.70 (0.54)
H-85	120.75 (9.29)	51.84 (6.19)	171.52	31.13 (3.50, 3.01)	Ne1 181.00 (7.76), Ne2 219.15, H δ 2 (6.91)
D-86	116.87 (8.09)	49.51 (5.12)	176.30	41.90 (3.44, 2.69)	
S-87	114.60 (9.14)	58.35	172.81		
L-88	121.08 (8.01)	52.56 (4.40)	175.45	39.42 (1.78, 1.58)	C γ 24.60 (1.49), C δ 1 22.70 (0.81), C δ 2 20.40 (0.77)
G-89	106.18 (7.80)	42.50 (4.27, 3.59)	173.07		
G-90	111.04 (8.47)	42.79 (3.98, 3.29)	172.20		
E-91	121.08 (7.98)	53.47 (5.40)	172.98	31.79 (1.81)	C γ 36.70 (1.96, 1.87)
I-92	120.75 (8.60)	56.25 (4.61)	170.37	40.36 (1.71)	C γ 1 25.00 (0.92), C γ 2 15.00 (0.68), C δ 13.10 (0.61)
L-93	123.34 (8.51)	51.67 (4.75)	172.58	41.29 (1.58, 0.96)	C γ 24.60 (1.53), C δ 1 22.50 (0.70), C δ 2 20.90 (0.69)
V-94	121.72 (8.82)	57.27 (4.72)	172.38	31.50 (0.35)	C γ 1 20.50 (0.39), C γ 2 19.40 (0.44)
T-95	113.30 (8.77)	56.60 (5.13)	170.52	68.54 (4.08)	C γ 19.00 (1.03)
Y-96	120.43 (8.46)	54.84 (4.83)	171.24	40.01 (2.77, 2.53)	H γ (6.95), H ζ (6.36), H η (6.26)
D-97	124.32 (7.61)	51.21 (4.74)	170.84	39.33 (2.53, 2.15)	
D-98	117.51 (6.04)	49.26 (4.54)	171.55	41.31 (2.41, 1.89)	
L-99	119.78 (9.02)	53.01 (4.10)	175.83	39.91(1.48, 1.41)	C γ 24.30 (1.59), C δ 1 22.60 (0.83), C δ 2 21.50 (0.81)
L-100	126.26 (8.57)	50.70 (4.23)		38.41 (1.48, 0.80)	C γ 24.00 (1.56), C δ 1 22.38 (0.09), C δ 2 20.59 (0.12)
P-101		60.12 (4.46)	174.95	29.61 (2.47, 1.95)	C γ 25.30 (2.13, 1.82), C δ 47.30 (3.65, 3.20)
D-102	122.05 (8.64)	54.68 (4.24)	174.95	38.21 (2.55)	
L-103	114.60 (7.82)	52.49 (4.08)	173.90	38.57 (1.63, 1.47)	C γ 24.40 (1.46), C δ 1 22.50 (0.70), C δ 2 20.50 (0.59)
F-104	119.13 (7.51)	57.46 (3.78)	172.75	37.52 (2.94, 2.52)	Cz (6.42), Cg (6.61), Hz (5.66)
R-105	126.58 (7.49)	51.81 (4.32)	171.95	31.23 (1.56, 1.37)	C γ 24.00 (1.51, 1.38), C δ 40.80 (3.13, 3.00)
E-106	120.75 (8.64)	55.22 (3.51)	174.56	28.23 (1.92, 1.81)	C γ 34.50 (2.37, 2.12)
G-107	111.04 (8.86)	42.88 (4.05, 3.67)	170.60		
Q-108	116.22 (7.19)	51.45 (4.55)	173.52	29.50 (2.00, 1.72)	C γ 31.50 (2.12), Ne 110.71 (7.29, 6.64)
G-109	108.44 (8.68)	43.77 (4.59, 3.60)	172.18		
I-110	118.49 (8.94)	56.08 (4.99)	172.09	42.13 (1.68)	C γ 1 24.40 (1.32, 0.82), C γ 2 18.20 (0.59), C δ 13.80 (0.73)
V-111	119.13 (8.54)	59.21 (4.90)	172.10	32.60 (1.77)	C γ 1 19.50 (0.86), C γ 2 19.00 (0.79)
A-112	128.20 (9.27)	47.07 (5.31)	172.59	19.64 (1.08)	
Q-113	119.78 (8.50)	51.27 (5.42)	173.06	30.16 (2.00, 1.92)	C γ 32.00 (2.19, 2.11), Ne 111.36 (7.33, 6.79)
G-114	110.71 (8.79)	44.23 (4.45, 4.32)			
V-115	118.49 (7.68)	58.19 (4.55)	173.93	32.19 (1.76)	C γ 1 19.00 (0.78), C γ 2 18.50 (0.66)
L-116	129.82 (8.36)	52.49 (4.27)	173.82	40.07 (1.76, 0.99)	C γ 24.00 (1.46), C δ 1 22.90 (0.43), C δ 2 20.60 (0.49)
G-117	114.28 (8.83)	42.55 (4.44, 3.93)			
E-118	121.08 (9.01)	56.36 (3.91)	173.96	26.94 (1.95, 1.88)	C γ 34.00 (2.19)
D-119	115.25 (8.02)	50.42 (4.33)	174.57	37.53 (2.88, 2.53)	
G-120	106.83 (7.75)	43.13 (4.08, 3.41)			
K-121	118.16 (7.47)	52.63 (4.58)	173.69	31.02 (1.63, 1.26)	C γ 22.90 (1.07), C δ 27.30 (1.39, 1.29), Ce 39.53 (2.76, 2.70)
L-122	125.29 (8.93)	51.54 (4.42)	171.32	41.92 (1.90, 0.86)	C γ 25.20 (0.93), C δ 1 23.50 (0.48), C δ 2 21.70 (0.42)
A-123	131.12 (8.32)	48.18 (4.81)	174.52	14.91 (1.24)	
A-124	128.20 (8.97)	50.33 (4.66)	175.27	17.24 (1.24)	
T-125	111.04 (9.65)	59.70 (4.51)	172.59	66.92 (4.37)	C γ 20.00 (1.19), Hg1 (6.46)
E-126	120.75 (7.73)	54.26 (4.77)	171.94	31.75 (1.99, 1.90)	C γ 34.50 (2.18, 2.00)

V-127	122.37 (8.04)	59.46 (4.35)	170.62	32.53 (1.269)	C γ 1 19.00 (0.55), C γ 2 17.70 (0.068)
L-128	125.29 (8.90)	50.88 (4.65)	173.53	42.11 (1.54, 1.45)	C γ 24.70 (1.40), C δ 1 22.80 (0.75), C δ 2 21.30 (0.79)
A-129	124.00 (8.57)	49.60 (4.38)	173.84	16.92 (1.06)	
K-130	122.70 (7.82)	52.59 (4.27)	172.67	31.32 (1.63, 1.33)	C γ 21.90 (1.20), C δ 26.56 (1.50), C ϵ 39.74 (2.77)
H-131	121.72 (8.40)	53.55 (4.58)	172.74	28.57 (3.02, 2.91)	Ne1 175.97 (6.92), Ne2 221.75, H δ 2 (7.77)
D-132	119.78 (8.25)	51.59 (4.42)	173.18	38.55 (2.48)	
E-133	118.81 (7.95)	53.73 (4.08)	172.89	28.48 (1.70, 1.61)	C γ 33.60 (1.98)
N-134	118.81 (8.16)	50.53 (4.58)	171.22	37.00 (2.58, 2.47)	N δ 112.66 (7.44, 6.73)
Y-135	124.96 (7.50)	56.94 (4.27)		37.50 (2.99, 2.63)	H γ (6.91), H ζ (7.02)

Allowed range for 30 ϕ , 20 ψ and 39 χ 1 angle constraints

37	PHE	PHI	-155	-85	37	PHE	PSI	60	175	68	VAL	CHI1	30	80
38	TYR	PHI	-155	-85	58	GLN	PSI	60	175	70	SER	CHI1	-100	-50
58	GLN	PHI	-155	-85	59	ARG	PSI	60	175	73	ARG	CHI1	30	80
59	ARG	PHI	-155	-85	60	ILE	PSI	60	175	74	ASP	CHI1	-100	-50
60	ILE	PHI	-155	-85	72	VAL	PSI	60	175	76	ASN	CHI1	-90	-40
61	ARG	PHI	-155	-85	73	ARG	PSI	60	175	77	SER	CHI1	-60	-10
72	VAL	PHI	-155	-85	80	VAL	PSI	60	175	78	LEU	CHI1	10	60
80	VAL	PHI	-155	-85	81	GLN	PSI	60	175	79	HIS	CHI1	-110	-60
81	GLN	PHI	-155	-85	82	PHE	PSI	60	175	80	VAL	CHI1	-120	-70
82	PHE	PHI	-155	-85	83	ALA	PSI	60	175	81	GLN	CHI1	30	80
83	ALA	PHI	-155	-85	84	VAL	PSI	60	175	82	PHE	CHI1	50	100
84	VAL	PHI	-155	-85	91	GLU	PSI	60	175	85	HIS	CHI1	50	100
85	HIS	PHI	-155	-85	92	ILE	PSI	60	175	86	ASP	CHI1	-170	-120
86	ASP	PHI	-155	-85	93	LEU	PSI	60	175	88	LEU	CHI1	-110	-50
92	ILE	PHI	-155	-85	94	VAL	PSI	60	175	93	LEU	CHI1	-110	-50
93	LEU	PHI	-155	-85	95	THR	PSI	60	175	97	ASP	CHI1	20	70
94	VAL	PHI	-155	-85	96	TYR	PSI	60	175	99	LEU	CHI1	-110	-60
95	THR	PHI	-155	-85	111	VAL	PSI	60	175	100	LEU	CHI1	-110	-60
96	TYR	PHI	-155	-85	122	LEU	PSI	60	175	102	ASP	CHI1	-100	-50
110	ILE	PHI	-155	-85	123	ALA	PSI	60	175	105	ARG	CHI1	-110	-60
111	VAL	PHI	-155	-85	36	LEU	CHI1	50	100	106	GLU	CHI1	-90	-40
112	ALA	PHI	-155	-85	37	PHE	CHI1	-100	-50	108	GLN	CHI1	40	90
113	GLN	PHI	-155	-85	42	GLU	CHI1	-170	-120	111	VAL	CHI1	-80	-30
121	LYS	PHI	-155	-85	45	ASN	CHI1	-80	-30	115	VAL	CHI1	30	80
122	LEU	PHI	-155	-85	47	LYS	CHI1	-100	-50	116	LEU	CHI1	-100	-50
123	ALA	PHI	-155	-85	52	VAL	CHI1	-100	-50	122	LEU	CHI1	-80	-30
125	THR	PHI	-155	-85	53	LYS	CHI1	-120	-60	127	VAL	CHI1	-90	-40
126	GLU	PHI	-155	-85	58	GLN	CHI1	-100	-50	128	LEU	CHI1	-60	-10
127	VAL	PHI	-155	-85	61	ARG	CHI1	-70	-20	130	LYS	CHI1	40	90
128	LEU	PHI	-155	-85	65	MET	CHI1	30	80					

Experimentally determined hydrogen bonds in apoCcmE

95 THR CO 124 ALA HN
 122 LEU CO 95 THR HN
 121 LYS CO 117 GLY HN
 115 VAL CO 123 ALA HN
 111 VAL CO 128 LEU HN
 124 GLY CO 60 ILE HN
 60 ILE CO 124 GLY HN
 122 ALA CO 62 VAL HN
 62 VAL CO 122 ALA HN
 61 ARG CO 38 TYR HN
 81 GLN CO 72 VAL HN
 96 TYR CO 80 VAL HN
 82 PHE CO 94 VAL HN
 94 VAL CO 82 PHE HN
 84 VAL CO 92 ILE HN

Experimental upper distance limites and NOE intensities

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.

30 LEU

HN 30 LEU HB2 5.16467
 HN 30 LEU HB3 5.63822
 HN 30 LEU HG 5.72871
 HN 30 LEU QD1 7 740
 HN 30 LEU QD2 7 656
 HB2 30 LEU HG 2.4557400
 HB2 30 LEU QD1 4.712080
 HB2 30 LEU QD2 4.615100
 HB3 30 LEU HG 2.6340900
 HB3 30 LEU QD1 5.26966
 HB3 30 LEU QD2 4.516710
 HG 30 LEU QD1 4.99464
 HG 30 LEU QD2 5 9248

31 ASN

HN 31 ASN HA 4.611720
 HA 31 ASN HB2 6 1060
 HA 31 ASN HB3 6 746
 HB2 31 ASN HD21 5.43947
 HB2 31 ASN HD22 5.43667
 HB3 31 ASN HD21 5.34056
 HB3 31 ASN HD22 5.24805

32 SER

HN 33 ASN HN 4.98316
 HA 32 SER HB2 3.835900
 HA 32 SER HB3 4 29160
 HA 33 ASN HN 5.25447

33 ASN

HN 33 ASN HA 2.9186900
 HN 33 ASN HB2 4.514080
 HN 33 ASN HB3 4.220560
 HA 33 ASN HB2 5.16112
 HA 33 ASN HB3 5.83014

34 LEU

HN 34 LEU HA 4.220380
 HN 34 LEU HB2 4 29880
 HN 34 LEU HB3 4.514290
 HN 34 LEU HG 4.78305
 HN 35 ASN HN 4.97992
 HA 34 LEU HB2 6 1411
 HA 34 LEU HB3 4.415700
 HA 34 LEU HG 4.78998
 HA 34 LEU QD1 4.129240
 HA 34 LEU QD2 4.99780
 HB2 34 LEU HG 5.82467
 HB2 34 LEU QD1 5.83607
 HB2 34 LEU QD2 5.45722
 HB2 35 ASN HA 4.612310
 HB3 34 LEU HG 4.216250
 HB3 34 LEU QD1 5.54703
 HB3 34 LEU QD2 5.45423
 HG 34 LEU QD1 6.12613
 HG 34 LEU QD2 5.54997
 QD2 35 ASN HA 6.85832

35 ASN

HN 35 ASN HA 4.317230
 HN 35 ASN HB3 4.612640
 HN 36 LEU HN 4.318800
 HA 35 ASN HB2 4.89682
 HA 35 ASN HB3 4 27810
 HA 35 ASN HD21 6 1385
 HA 35 ASN HD22 5.43643
 HA 36 LEU HN 3.934640
 HB2 35 ASN HD21 5.43851
 HB2 35 ASN HD22 5.24992
 HB3 35 ASN HD21 5 6159
 HB3 35 ASN HD22 4.78945
 HB3 36 LEU HN 5.26050

36 LEU

HN 36 LEU HA 4 27870
 HN 36 LEU HB2 4 27510
 HN 36 LEU HB3 4.89429
 HN 36 LEU HG 4.316120
 HN 36 LEU QD1 5.74024
 HN 36 LEU QD2 5.35954

HN	37 PHE	HN	5.54311	CZ	61 ARG	QD	9	367.5*4
HN	60 ILE	HA	4.38909	CZ	113 GLN	HE2	7.4	
HN	60 ILE	QG2	7 1062	24040.0*2				
HN	61 ARG	HN	3.533950	CZ	128 LEU	QD1	9	
HA	36 LEU	HB2	4.514320	590.0*2				
HA	36 LEU	HB3	4.123650	CZ	128 LEU	QD2	9	
HA	36 LEU	QB	7 2112.0*2	1042.0*2				
HA	36 LEU	HG	4.87834	HZ	61 ARG	HG2	6 3365	
HA	36 LEU	QD1	5.93308	HZ	111 VAL	QG1	7 3930	
HA	36 LEU	QD2	4.810810	HZ	111 VAL	QG2	7 1411	
HA	37 PHE	HN	3.1133000	HZ	113 GLN	HE2	6 1114	
HB2	36 LEU	QD1	4.811380	38 TYR				
HB2	36 LEU	QD2	4.224820	HN	38 TYR	HA	3.933820	
HB2	37 PHE	HN	5.83072	HN	38 TYR	HB2	3.649820	
HB3	36 LEU	HG	4.121660	HN	38 TYR	HB3	4.88990	
HB3	36 LEU	QD1	4.712670	HN	38 TYR	CG	7.9 2289.0*2	
HB3	36 LEU	QD2	5.45531	HN	38 TYR	CZ	7 381.0*2	
QB	36 LEU	HG	6.2	HN	39 THR	HN	6 2198	
4810.0*2				HN	61 ARG	HN	3.821260	
QB	36 LEU	QD1	7.1 2635.5*2	HN	62 VAL	HA	3.346350	
QB	36 LEU	QD2	5 35200.0*2	HN	63 GLY	HN	3.627440	
QB	37 PHE	HN	6.2 5890.0*2	HA	38 TYR	HB2	5.73393	
HG	36 LEU	QD1	5 8525	HA	38 TYR	HB3	4.415340	
HG	36 LEU	QD2	4.420110	HA	38 TYR	CG	7 1167.5*2	
HG	37 PHE	HN	6 4497	HA	39 THR	HN	3.482660	
HG	38 TYR	CG	8 329.5*2	HB2	38 TYR	CG	6.2 16320.0*2	
QD1	37 PHE	HN	6.76296	HB2	38 TYR	CZ	8 1618.5*2	
QD1	38 TYR	CG	9 487.0*2	HB2	39 THR	HN	6 1509	
QD2	37 PHE	HN	7 1826	HB2	43 ILE	QD1	7 2266	
QD2	38 TYR	CG	9 339.0*2	HB3	38 TYR	CG	6.6 10070.0*2	
QD2	60 ILE	HB	5 26860	HB3	38 TYR	CZ	8 1981.0*2	
QD2	60 ILE	QG2	6.222430	HB3	39 THR	HN	4.711320	
37 PHE				HB3	43 ILE	QD1	7 2557	
HN	37 PHE	HA	3.653410	CG	38 TYR	CZ	7.7 40225.0*4	
HN	37 PHE	HB2	4.220150	CG	39 THR	HN	8 258.0*2	
HN	37 PHE	HB3	4.416300	CG	42 GLU	HB2	8 3141.5*2	
HN	37 PHE	CG	6.6 9645.0*2	CG	60 ILE	HB	8 1377.5*2	
HA	37 PHE	HB2	4.318880	CG	60 ILE	QG2	9 991.0*2	
HA	37 PHE	HB3	3.931720	CG	60 ILE	QD1	9 1511.5*2	
HA	37 PHE	CG	7 1711.0*2	39 THR				
HA	38 TYR	HN	3.2105600	HN	39 THR	HA	4.612430	
HA	61 ARG	HN	3.439310	HN	39 THR	HB	4.611500	
HA	61 ARG	HB2	6 13720	HN	39 THR	QG2	4.322230	
HA	61 ARG	HB3	6 3468	HN	42 GLU	HN	6 2566	
HA	61 ARG	HG2	6 2266	HN	42 GLU	HB3	5.310170	
HA	61 ARG	HG3	6 2977	HA	39 THR	HB	3.396220	
HA	61 ARG	QD	7 835.5*2	HA	39 THR	QG2	3.665570	
HB2	37 PHE	CG	6.5 10770.0*2	HA	40 PRO	HG2	6 924	
HB2	37 PHE	CZ	8 1030.0*2	HA	40 PRO	HG3	6 1239	
HB2	38 TYR	HN	5.92634	HA	40 PRO	HD2	5.620390	
HB2	61 ARG	HB3	6 2979	HA	40 PRO	HD3	4.759840	
HB2	61 ARG	HG3	6 2116	HA	62 VAL	QG1	7 1755	
HB3	37 PHE	CG	7.2 5030.0*2	HA	63 GLY	HN	3.533680	
HB3	37 PHE	CZ	8 1490.0*2	HB	39 THR	QG2	3.4104700	
HB3	38 TYR	HN	5.63621	HB	40 PRO	HD2	5.230890	
HB3	61 ARG	HB2	6 2457	HB	40 PRO	HD3	6 9279	
HB3	61 ARG	HB3	6 2550	HB	41 SER	HN	6 2232	
CG	37 PHE	CZ	7.3 78325.0*4	HB	86 ASP	HB3	6 3023	
CG	37 PHE	HZ	5.3 76350.0*2	QG2	40 PRO	HG2	7 1314	
CG	61 ARG	HB2	8 731.0*2	QG2	40 PRO	HD2	7 1120	
CG	61 ARG	QD	9 190.8*4	QG2	40 PRO	HD3	6.57322	
CZ	37 PHE	HZ	6 24785.0*2	QG2	42 GLU	HN	6.110440	

40	QG2	42	GLU	HB2	7	3098	HA	44	VAL	HN	5.76833
PRO							HA	44	VAL	HB	4.917330
	HA	40	PRO	QB	6	7110.0*2	HA	44	VAL	QG1	5.911600
	HA	40	PRO	HG2	6	703	HA	44	VAL	QG2	7 3845
	HA	40	PRO	HG3	6	1762	HA	45	ASN	HD21	6 1528
	HA	40	PRO	HD2	4	23720	HA	45	ASN	HD22	6 814
	HA	40	PRO	HD3	4.6	10570	HA	88	LEU	QD1	6.76094
	HA	41	SER	HN	4.5	14100	HA	90	GLY	HN	5.61883
	HA	42	GLU	HN	6	4862	HA	90	GLY	HA1	3.819000
	HA	43	ILE	HN	5.4	9998	HA	90	GLY	HA2	4.66114
	HA	43	ILE	QG2	7	2602	HB2	42	GLU	HN	4.221150
	HA	43	ILE	HG12	6	2150	HB2	43	ILE	HN	5 15790
	HA	43	ILE	HG13	6	2602	HB2	44	VAL	QG1	7 2172
	HA	43	ILE	QD1	5.4	18320	HB2	45	ASN	HD21	6 1251
	HA	62	VAL	QG1	7	3353	HB2	90	GLY	HA2	6 1911
	HA	62	VAL	QG2	7	1686	HB3	42	GLU	HN	4.98645
	HA	92	ILE	QG2	6.3	8909	HB3	45	ASN	HD21	6 1566
	QB	40	PRO	HG2	4.9	27480.0*2	HB3	86	ASP	HB2	6 1614
	QB	40	PRO	HG3	5.6	9645.0*2	HB3	88	LEU	QD1	6.57084
	QB	40	PRO	HD2	6.2	4891.0*2	HB3	90	GLY	HA2	6 1097
	QB	41	SER	HN	5.4	14940.0*2					
	QB	43	ILE	HG12	7	1761.0*2	HN	42	GLU	HA	4.219870
	QB	43	ILE	HG13	7	5255.0*2	HN	42	GLU	HB2	4.710220
	QB	43	ILE	QD1	8	825.0*2	HN	42	GLU	HB3	4 28310
	QB	62	VAL	QG1	8	1721.0*2	HN	42	GLU	HG2	4.314610
	QB	62	VAL	QG2	8	3597.0*2	HN	42	GLU	HG3	5 6253
	QB	84	VAL	QG2	8	1295.0*2	HN	43	ILE	HN	3.1128500
	QB	85	HIS	HA	7	342.5*2	HN	43	ILE	HG12	6 1455
	QB	91	GLU	HA	7	1445.5*2	HA	42	GLU	HB2	4.89952
	QB	92	ILE	HN	7	1510.0*2	HA	42	GLU	HB3	5.83072
	QB	92	ILE	QG2	7.3	8675.0*2	HA	42	GLU	HG2	5.92214
	HG2	40	PRO	HD2	5.4	3705	HA	42	GLU	HG3	4.96691
	HG2	40	PRO	HD3	4.1	20200	HA	43	ILE	HN	5.82907
	HG2	41	SER	HN	6	2434	HA	44	VAL	HN	6 1141
	HG2	62	VAL	QG2	6.8	5985	HA	45	ASN	HN	5.49691
	HG2	84	VAL	QG1	6	10860	HB2	42	GLU	HG2	3.927150
	HG2	84	VAL	QG2	5.9	11840	HB2	42	GLU	HG3	3.734690
	HG2	85	HIS	HA	6	5178	HB2	43	ILE	HN	5.92772
	HG3	40	PRO	HD2	5.1	5266	HB2	43	ILE	QD1	7 4094
	HG3	40	PRO	HD3	4	21820	HB3	42	GLU	HG2	2.8184800
	HG3	41	SER	HN	6	5142	HB3	42	GLU	HG3	5.62944
	HG3	62	VAL	QG1	6.6	6741	HB3	43	ILE	HN	5.54262
	HG3	62	VAL	QG2	6.6	6733	HG2	43	ILE	HN	6 2403
	HG3	84	VAL	QG2	5.6	15350	HG3	47	LYS	HA	6 899
	HD2	41	SER	HN	6	8438					
	HD2	42	GLU	HB2	6	12150	HN	43	ILE	HA	3.841510
	HD2	62	VAL	QG2	7	1331	HN	43	ILE	HB	3.933110
	HD2	64	GLY	HA2	6	1460	HN	43	ILE	QG2	4.810720
	HD3	41	SER	HN	6	585	HN	43	ILE	HG12	4.216530
	HD3	62	VAL	QG2	6.5	7205	HN	43	ILE	HG13	4 25210
41	SER						HN	43	ILE	QD1	5.36383
	HN	41	SER	HA	4.1	25580	HN	44	VAL	HN	3.748800
	HN	41	SER	HB2	4.6	12930	HN	44	VAL	QG1	7 1045
	HN	41	SER	HB3	4.1	23110	HN	45	ASN	HN	6 1100
	HN	42	GLU	HN	3.7	43780	HA	43	ILE	HB	4.319230
	HN	43	ILE	HN	6	1507	HA	43	ILE	QG2	4.226590
	HN	90	GLY	HN	5.8	1546	HA	43	ILE	HG12	4.218480
	HN	90	GLY	HA2	5.9	1435	HA	43	ILE	HG13	3.642980
	HA	41	SER	HB2	3	149600	HA	43	ILE	QD1	5.45621
	HA	41	SER	HB3	3.2	117600	HA	44	VAL	HN	4.97785
	HA	42	GLU	HN	4.4	15690	HA	45	ASN	HN	6 531
	HA	43	ILE	HN	4.9	17110	HA	47	LYS	QG	7 3638.5*2

HA	48 THR	HB	6	842	HN	46 GLY	HN	4.221280
HA	54 PRO	HD2	6	3828	HN	47 LYS	HN	6 2879
HB	43 ILE	QG2	4.1	30430	HN	47 LYS	HB2	6 4408
HB	43 ILE	HG12	2.9	160700	HN	49 ASP	QB	7 3479.0*2
HB	43 ILE	HG13	3.2	93580	HA	45 ASN	HB2	4.98408
HB	43 ILE	QD1	4.4	19690	HA	45 ASN	HB3	4 26910
HB	44 VAL	HN	4.6	12270	HA	46 GLY	HN	5.44793
HB	48 THR	HB	6	3665	HB2	45 ASN	HD21	3.829500
HB	92 ILE	QG1	7	3386.5*2	HB2	45 ASN	HD22	4.314840
QG2	43 ILE	HG12	4.4	19680	HB2	46 GLY	HN	4.416360
QG2	43 ILE	HG13	3.4	855600	HB3	45 ASN	HD21	3.548510
QG2	43 ILE	QD1	4.5	72620	HB3	45 ASN	HD22	4.511400
QG2	44 VAL	HN	6.9	5588	HB3	46 GLY	HN	4.513040
QG2	47 LYS	HB3	7	3669	HD21	46 GLY	HN	6 665
QG2	47 LYS	HD2	7	2124	46 GLY			
QG2	54 PRO	HD2	7	1466	HN	46 GLY	HA1	3.559320
QG2	54 PRO	HD3	6.8	5888	HN	46 GLY	HA2	3.656800
HG12	43 ILE	QD1	3.4	126900	HN	47 LYS	HN	5.16530
HG12	44 VAL	HN	6	662	HN	50 THR	HN	6 3671
HG12	62 VAL	QG1	6.8	5833	HA1	47 LYS	HN	3.653720
HG12	62 VAL	QG2	6	11330	HA1	50 THR	HN	6 2005
HG13	43 ILE	QD1	4.3	21460	HA1	50 THR	HB	6 5040
HG13	44 VAL	HN	6	3874	HA1	53 LYS	HG3	6 1235
QD1	44 VAL	HN	7	1339	HA2	47 LYS	HN	3.567960
QD1	60 ILE	QD1	5	81240	HA2	52 VAL	QG2	7 3106
QD1	62 VAL	HB	6.2	9612	HA2	53 LYS	HG3	6 492
QD1	62 VAL	QG1	5.4	55470	47 LYS			
44 VAL					HN	47 LYS	HA	4.97764
HN	44 VAL	HA	3.9	30800	HN	47 LYS	HB2	4 27320
HN	44 VAL	HB	3.8	41010	HN	47 LYS	HB3	3.837430
HN	44 VAL	QG1	4.5	17540	HN	47 LYS	QG	5.8 7715.0*2
HN	44 VAL	QG2	5.2	6580	HN	47 LYS	HD2	6 1696
HN	45 ASN	HN	3.4	81150	HN	47 LYS	HD3	5.24664
HN	45 ASN	HD22	5.1	35770	HN	48 THR	HN	4.122820
HN	46 GLY	HN	6	1025	HN	50 THR	HN	6 1376
HA	44 VAL	HB	4.2	21560	HN	51 GLY	HN	6 416
HA	44 VAL	QG1	3.6	60590	HN	52 VAL	HN	3.916490
HA	44 VAL	QG2	3.9	40950	HN	52 VAL	QG1	7 1148
HA	45 ASN	HN	5	7191	HN	52 VAL	QG2	7 1470
HA	92 ILE	QD1	7	3833	HA	47 LYS	HB2	4.89197
HB	44 VAL	QG1	4.2	25470	HA	47 LYS	HB3	4.98575
HB	44 VAL	QG2	4	31540	HA	47 LYS	QG	4.9 15445.0*2
HB	45 ASN	HN	4.7	10060	HA	47 LYS	HD2	5.24936
HB	45 ASN	HD22	5.5	21680	HA	47 LYS	HD3	4.510690
HB	92 ILE	HB	6	8510	HA	47 LYS	HE3	6 952
HB	92 ILE	QD1	6.4	7685	HA	48 THR	HN	4.219910
QG1	45 ASN	HN	5.3	20940	HA	49 ASP	HN	6 2116
QG1	45 ASN	HD21	7	1385	HA	50 THR	HN	6 1581
QG1	45 ASN	HD22	6.3	8691	HB2	47 LYS	QG	5.4 13005.0*2
QG1	47 LYS	HN	7	2121	HB2	47 LYS	HD2	6 1169
QG1	91 GLU	HN	7	2346	HB2	47 LYS	HD3	5.34286
QG2	45 ASN	HN	6.1	10220	HB2	47 LYS	HE2	4.97092
QG2	45 ASN	HD21	7	4008	HB2	47 LYS	HE3	4.511450
QG2	45 ASN	HD22	6.5	7384	HB2	48 THR	HN	5.44486
QG2	91 GLU	HN	7	1299	HB2	49 ASP	HN	5.58904
QG2	92 ILE	QD1	5.9	31090	HB2	50 THR	HN	6 4070
45 ASN					HB2	51 GLY	HN	6 4617
HN	45 ASN	HA	3.7	48980	HB2	52 VAL	HN	6 2510
HN	45 ASN	HB2	4.3	17860	HB2	54 PRO	HG3	6 515
HN	45 ASN	HB3	4.2	20550	HB3	47 LYS	QG	5.6 10415.0*2
HN	45 ASN	HD21	4.4	13360	HB3	47 LYS	HD2	4.512000
HN	45 ASN	HD22	6	1102	HB3	47 LYS	HD3	5 6279

HB3	47	LYS	HE2	6	578	HN	50	THR	HA	3.934500
HB3	48	THR	HN	5.25617		HN	50	THR	HB	4.513120
HB3	48	THR	HA	6	2346	HN	50	THR	QG2	4.811090
HB3	48	THR	HB	6	1300	HN	51	GLY	HN	3.470610
HB3	50	THR	HN	6	2238	HN	52	VAL	HN	6 3207
HB3	52	VAL	HN	6	2829	HA	50	THR	HB	3.565670
QG	47	LYS	HD2	4.5	51350.0*2	HA	50	THR	QG2	3.573430
QG	47	LYS	HD3	5.8	7680.0*2	HA	51	GLY	HN	3.655460
QG	47	LYS	HE2	7	0.0*2	HA	51	GLY	HA1	5.82911
QG	47	LYS	HE3	6.2	4576.5*2	HA	51	GLY	HA2	6 2462
QG	48	THR	HN	7	269.0*2	HA	52	VAL	HN	6 2126
QG	49	ASP	HN	7	4016.5*2	HA	52	VAL	QG1	7 2351
QG	50	THR	HN	7	1410.5*2	HA	52	VAL	QG2	7 2490
QG	54	PRO	HG3	7	5430.0*2	HB	50	THR	QG2	3.4121600
HD2	47	LYS	HE2	5.15517		HB	51	GLY	HN	4.123720
HD2	47	LYS	HE3	5	6400	HB	52	VAL	HN	5.86305
HD2	53	LYS	HB2	6	3442	HB	52	VAL	HA	6 3685
HD3	47	LYS	HE2	4.315190		HB	52	VAL	HB	6 3321
HD3	47	LYS	HE3	4.69815		HB	52	VAL	QG1	6.66974
HD3	48	THR	HN	6	756	HB	52	VAL	QG2	6.66974
HE2	53	LYS	HB2	6	1075	QG2	51	GLY	HN	5.911430
48 THR						QG2	51	GLY	HA2	7 2317
HN	48	THR	HA	3.746600		QG2	52	VAL	HN	6.76431
HN	48	THR	HB	3.838340		QG2	52	VAL	HB	5.911530
HN	48	THR	QG2	4.811590		QG2	52	VAL	QG1	5.738490
HN	49	ASP	HN	4.612790		QG2	52	VAL	QG2	5.738770
HN	50	THR	HN	6	1672	51 GLY				
HA	48	THR	HB	3.838420		HN	51	GLY	HA1	3.469580
HA	48	THR	QG2	4 31710		HN	51	GLY	HA2	3.744130
HA	49	ASP	HN	3.838010		HN	52	VAL	HN	3.841190
HA	49	ASP	HA	5 7326		HN	52	VAL	HA	5.92574
HA	50	THR	HN	5.113020		HN	53	LYS	HN	6 3881
HA	51	GLY	HA1	4.819650		HA1	52	VAL	HN	4.415930
HA	51	GLY	HA2	4.624710		HA2	52	VAL	HN	5 7215
HA	52	VAL	HN	6 4956		HA2	54	PRO	HG2	6 4862
HA	56	ALA	HA	6 1286		HA2	54	PRO	HD2	6 1145
HB	48	THR	QG2	5.55130		52 VAL				
HB	49	ASP	HN	5.73297		HN	52	VAL	HA	3.748380
HB	50	THR	HN	6 4090		HN	52	VAL	HB	4.319180
QG2	49	ASP	HN	6.110420		HN	52	VAL	QG1	4.322940
QG2	49	ASP	HA	6.29010		HN	52	VAL	QG2	4.131320
QG2	49	ASP	QB	8 1491.5*2		HN	53	LYS	HN	6 2528
QG2	50	THR	HN	7 869		HN	53	LYS	HB2	6 872
QG2	92	ILE	QG1	6.8 12935.0*2		HA	52	VAL	HB	4.220930
QG2	92	ILE	QD1	7 10800		HA	52	VAL	QG1	4.614630
QG2	116	LEU	QD1	6 27380		HA	52	VAL	QG2	5 8811
QG2	120	GLY	HN	7 1674		HA	53	LYS	HN	3.658010
QG2	120	GLY	HA1	7 1281		HA	53	LYS	HG3	6 1672
49 ASP						HA	53	LYS	QD	7 168.0*2
HN	49	ASP	HA	3.748480		HB	52	VAL	QG1	4.322270
HN	49	ASP	QB	4.9 17200.0*2		HB	52	VAL	QG2	4.418650
HN	50	THR	HN	4 30510		HB	53	LYS	HN	6 1299
HN	51	GLY	HN	6 2640		QG1	53	LYS	HN	4.269980
HA	49	ASP	QB	4.1 59450.0*2		QG2	53	LYS	HN	6 10560
HA	50	THR	HN	4.612910		QG2	53	LYS	HA	7 1832
HA	51	GLY	HN	6 1857		QG2	53	LYS	HG3	5 28400
HA	51	GLY	HA2	6 3878		53 LYS				
HA	92	ILE	QG1	7 940.0*2		HN	53	LYS	HA	4 27630
HA	120	GLY	HA1	5.61957		HN	53	LYS	HB2	5.35223
QB	50	THR	HN	5.7 11035.0*2		HN	53	LYS	HB3	4.124410
QB	50	THR	QG2	8 3721.0*2		HN	53	LYS	HG2	4.69452
50 THR						HN	53	LYS	HG3	4.511870

HN	53	LYS	QD	6.4	3721.0*2		HG3	54	PRO	HD3	3.927180
HN	53	LYS	HE2	6	1272		HG3	55	GLU	HN	5.915000
HN	54	PRO	HD2	6	5843	55	GLU				
HN	54	PRO	HD3	6	544		HN	55	GLU	HA	4 28290
HA	53	LYS	HB2	4.8	9643		HN	55	GLU	HB2	4.612880
HA	53	LYS	HB3	6	1897		HN	55	GLU	HB3	3.932280
HA	53	LYS	HG2	4.9	6879		HN	55	GLU	QG	5.2 16300.0*2
HA	53	LYS	HG3	5.1	5627		HN	56	ALA	HN	4.97828
HA	53	LYS	QD	5.3	14975.0*2		HN	58	GLN	HB2	5.67876
HA	53	LYS	HE3	4.8	7862		HN	58	GLN	HB3	6 4089
HA	54	PRO	HD2	4.8	49920		HN	58	GLN	HG3	6 5411
HA	54	PRO	HD3	5.4	24550		HN	58	GLN	HE21	5.717930
HB2	53	LYS	HG2	3.9	28840		HN	58	GLN	HE22	6 3527
HB2	53	LYS	HG3	4.5	11930		HA	55	GLU	HB2	3.656410
HB2	53	LYS	QD	6.5	3515.5*2		HA	55	GLU	HB3	4.124760
HB2	53	LYS	HE2	5.1	5189		HA	55	GLU	QG	4.4 31890.0*2
HB2	54	PRO	HD2	6	7792		HA	56	ALA	HN	3.835770
HB2	54	PRO	HD3	6	2377		HA	56	ALA	HA	6 1608
HB3	53	LYS	HG2	3.6	42490		HA	56	ALA	QB	5.91331
HB3	53	LYS	HG3	4.3	14560		HB2	55	GLU	QG	4.4 64600.0*2
HB3	53	LYS	QD	4.5	56550.0*2		HB2	56	ALA	HN	4.513750
HB3	53	LYS	HE2	4.8	7461		HB2	56	ALA	QB	6.66578
HB3	54	PRO	HB3	6	11120		HB2	58	GLN	HE22	6 4806
HB3	54	PRO	HG2	6	5381		HB3	55	GLU	QG	4.1 103800.0*2
HB3	54	PRO	HD2	6	5184		HB3	56	ALA	HN	4.319120
HB3	54	PRO	HD3	6	1692		HB3	58	GLN	HG2	6 1379
HG2	53	LYS	QD	4.4	59450.0*2		HB3	58	GLN	HG3	6 921
HG2	53	LYS	HE2	5.4	3595		HB3	58	GLN	HE21	6 3305
HG2	53	LYS	HE3	5.5	3280		HB3	58	GLN	HE22	6 4130
HG3	53	LYS	QD	5.7	8995.0*2		QG	56	ALA	HN	7 5620.0*2
HG3	53	LYS	HE2	4.6	10340		QG	58	GLN	HE21	7 5810.0*2
HG3	53	LYS	HE3	6	838		QG	58	GLN	HE22	7 1480.5*2
QD	53	LYS	HE2	5.3	15445.0*2	56	ALA				
54	PRO					HN	56	ALA	HA	3.742910	
HA	54	PRO	HB2	4.6	12060	HN	56	ALA	QB	3.483750	
HA	54	PRO	HB3	4.2	20700	HN	57	GLY	HN	5.16612	
HA	54	PRO	HG2	4	22880	HN	116	LEU	QD2	7 1604	
HA	54	PRO	HG3	4.5	11140	HA	56	ALA	QB	3.481940	
HA	54	PRO	HD3	6	1021	HA	57	GLY	HN	3.1129600	
HA	55	GLU	HN	3.8	39160	HA	57	GLY	HA1	6 2457	
HA	55	GLU	QG	7	782.0*2	HA	57	GLY	HA2	6 1289	
HA	58	GLN	HE21	6	2718	HA	58	GLN	HN	6 2374	
HA	58	GLN	HE22	6	1257	HA	116	LEU	HB2	6 3525	
HA	60	ILE	QG2	7	1590	HA	116	LEU	HG	6 5002	
HB2	54	PRO	HG2	3.5	48490	HA	116	LEU	QD1	7 3107	
HB2	54	PRO	HG3	3.4	59610	HA	116	LEU	QD2	7 3059	
HB2	54	PRO	HD2	6	991	HA	122	LEU	QD2	7 2650	
HB2	54	PRO	HD3	5.4	3913	QB	57	GLY	HN	4 14230	
HB2	55	GLU	HN	4.5	13560	QB	58	GLN	HN	5.71373	
HB2	55	GLU	QG	7	7125.0*2	QB	116	LEU	HA	7 1126	
HB2	60	ILE	QD1	7	4178	QB	116	LEU	HB2	7 706	
HB3	54	PRO	HG2	3.6	44310	QB	117	GLY	HA2	6.110430	
HB3	54	PRO	HG3	3.6	45860	QB	118	GLU	HN	7 809	
HB3	54	PRO	HD2	5.1	5138	QB	118	GLU	HA	5.714160	
HB3	54	PRO	HD3	4.7	9245	QB	118	GLU	HB2	7 879	
HB3	55	GLU	HN	5.4	4492	QB	118	GLU	QG	7	
HB3	60	ILE	QD1	6.6	6668	10520.0*2					
HG2	54	PRO	HD2	4.1	21120	QB	119	ASP	HN	7 1105	
HG2	54	PRO	HD3	4.6	9672	QB	120	GLY	HN	7 3254	
HG2	55	GLU	HN	6	9324	57	GLY				
HG2	60	ILE	QD1	6.7	6279	HN	57	GLY	HA1	3.396560	
HG3	54	PRO	HD2	4.7	8308	HN	57	GLY	HA2	3.838170	

HN	58 GLN	HN	3.474940
HN	115 VAL	QG2	5.517570
HN	116 LEU	HB2	6 7269
HN	116 LEU	HB3	6 2360
HN	122 LEU	QD2	7 1214
HA1	58 GLN	HN	4.513940
HA1	115 VAL	QG2	5.615460
HA2	58 GLN	HN	3.649700
HA2	115 VAL	QG2	6 10680

58 GLN

HN	58 GLN	HA	3.653400
HN	58 GLN	HB2	3.743970
HN	58 GLN	HB3	4.317360
HN	58 GLN	HG2	4.217500
HN	58 GLN	HG3	3.831790
HN	58 GLN	HE21	5.15586
HN	59 ARG	HN	4.89320
HN	115 VAL	HB	6 5221
HN	115 VAL	QG2	7 5030
HN	116 LEU	HN	4.113340
HN	116 LEU	HB2	6 2478
HN	116 LEU	HB3	6 524
HN	122 LEU	QD2	7 917
HA	58 GLN	HB2	4.124480
HA	58 GLN	HB3	4.125140
HA	58 GLN	HG2	4.118690
HA	58 GLN	HG3	4.315130
HA	59 ARG	HN	3.478360
HA	60 ILE	QG2	6.19828
HA	115 VAL	QG2	7 2823
HB2	58 GLN	HG2	3.461580
HB2	58 GLN	HG3	3.465910
HB2	58 GLN	HE21	5.63192
HB2	59 ARG	HN	4.710200
HB2	60 ILE	QG2	6.38307
HB3	58 GLN	HG2	3.379740
HB3	58 GLN	HG3	3.550610
HB3	58 GLN	HE21	6 1787
HB3	58 GLN	HE22	6 957
HB3	59 ARG	HN	4.79984
HB3	60 ILE	QG2	6.95335
HG2	58 GLN	HE21	3.740650
HG2	58 GLN	HE22	4.314150
HG3	58 GLN	HE21	4.120540
HG3	58 GLN	HE22	4.314380
HG3	59 ARG	HN	6 3846
HG3	60 ILE	QG2	7 2644
HE21	60 ILE	QG2	7 1450
HE22	60 ILE	QG2	7 2411

59 ARG

HN	59 ARG	HA	3.558630
HN	59 ARG	HB2	3.935050
HN	59 ARG	HB3	3.931020
HN	59 ARG	HG2	4.413960
HN	59 ARG	HG3	5.63132
HN	59 ARG	QD	7 1141.0*2
HN	60 ILE	HN	5.44411
HN	115 VAL	QG2	6.29441
HA	59 ARG	HB2	4.125060
HA	59 ARG	HB3	4.221300
HA	59 ARG	HG2	4.218030
HA	59 ARG	HG3	4.511660

HA	59 ARG	QD	7 541.0*2
HA	60 ILE	HN	3.653050
HA	115 VAL	HA	3.440410
HA	115 VAL	QG1	7 4629
HA	115 VAL	QG2	7 4493
HA	116 LEU	HN	3.533880
HB2	59 ARG	HG2	4.315710
HB2	59 ARG	HG3	3.833660
HB2	59 ARG	QD	6.1 5635.0*2
HB2	60 ILE	HN	5.16180
HB2	115 VAL	HA	6 2871
HB2	115 VAL	HB	4.667540
HB2	115 VAL	QG1	6.29362
HB3	59 ARG	HG2	4.120340
HB3	59 ARG	HG3	3.548780
HB3	59 ARG	QD	5.7 9290.0*2
HB3	60 ILE	HN	5.63793
HB3	115 VAL	HA	6 938
HG2	59 ARG	QD	4.8 34215.0*2
HG2	60 ILE	HN	6 7654
HG2	115 VAL	HA	6 1015
HG2	115 VAL	HB	5.620370
HG2	115 VAL	QG1	5.319700
HG3	59 ARG	QD	4.7 36560.0*2
HG3	60 ILE	HN	6 10640
QD	113 GLN	HE2	7

926.0*2

QD

3907.5*2

60 ILE

HN	60 ILE	HA	3.746580
HN	60 ILE	HB	4.317090
HN	60 ILE	QG2	4.323120
HN	60 ILE	HG12	4.610580
HN	60 ILE	HG13	4.216550
HN	60 ILE	QD1	5.27306
HN	61 ARG	HN	6 751
HN	114 GLY	HN	3.345040
HN	115 VAL	HA	3.345760
HA	60 ILE	HB	3.748830
HA	60 ILE	QG2	3.847800
HA	60 ILE	HG12	6 1276
HA	60 ILE	HG13	4.69744
HA	60 ILE	QD1	5.93236
HA	61 ARG	HN	3.1135200
HB	60 ILE	QG2	3.497650
HB	60 ILE	HG12	3.833160
HB	60 ILE	HG13	3.926810
HB	60 ILE	QD1	4.128570
HB	61 ARG	HN	3.933620
HB	116 LEU	QD2	7 2751
QG2	60 ILE	HG12	4.417920
QG2	60 ILE	HG13	3.484200
QG2	60 ILE	QD1	4.4101000
QG2	61 ARG	HN	5.517350
QG2	116 LEU	HN	7 3016
HG12	60 ILE	QD1	3.4103000
HG12	61 ARG	HN	6 6474
HG12	116 LEU	QD2	6.85793
HG13	60 ILE	QD1	3.660650
HG13	62 VAL	HN	6 2130
QD1	61 ARG	HN	7 5062

	QD1	62 VAL	HB	6.76070		HN	62 VAL	HA	3.935010
	QD1	62 VAL	QG1	6.222040		HN	62 VAL	HB	4.319210
	QD1	62 VAL	QG2	7.110360		HN	62 VAL	QG1	5.26571
	QD1	116 LEU	HN	7 2261		HN	62 VAL	QG2	4.417980
	QD1	116 LEU	HB3	7 4505		HN	63 GLY	HN	6 901
	QD1	116 LEU	QD1	5.737470		HN	111 VAL	HA	6 801
	QD1	116 LEU	QD2	5.643700		HN	111 VAL	QG1	7 2667
	QD1	122 LEU	QD1	6.418770		HN	112 ALA	HN	3.350400
61 ARG						HN	112 ALA	QB	6.57065
	HN	61 ARG	HA	4 26460		HN	113 GLN	HA	3.532700
	HN	61 ARG	HB2	3.748680		HA	62 VAL	HB	3.930540
	HN	61 ARG	HB3	3.933130		HA	62 VAL	QG1	3.845890
	HN	61 ARG	HG2	6 1403		HA	62 VAL	QG2	4 33060
	HN	61 ARG	HG3	3.646340		HA	63 GLY	HN	3.566630
	HN	61 ARG	QD	7 0.0*2		HB	62 VAL	QG1	4.517240
	HN	62 VAL	HN	6 903		HB	62 VAL	QG2	3.4125500
	HA	61 ARG	HB2	4.317560		HB	63 GLY	HN	4.97792
	HA	61 ARG	HB3	4.123580		QG1	63 GLY	HN	5.615260
	HA	61 ARG	HG2	4.511800		QG1	64 GLY	HN	6.85952
	HA	61 ARG	HG3	4 21760		QG1	112 ALA	HN	7 3820
	HA	61 ARG	QD	7 827.5*2		QG2	63 GLY	HN	5.417940
	HA	62 VAL	HN	3 152000		QG2	94 VAL	QG2	5.544670
	HA	113 GLN	HA	3.257020		QG2	104 PHE	CG	9
	HA	113 GLN	HB3	6 757	747.0*2				
	HA	113 GLN	HG2	6 1687		QG2	112 ALA	QB	5.545200
	HA	114 GLY	HN	3.819880	63 GLY				
	HB2	61 ARG	HG2	4.88156		HN	63 GLY	HA1	3.568810
	HB2	61 ARG	HG3	3.927700		HN	63 GLY	HA2	4 26660
	HB2	61 ARG	QD	5.7 8430.0*2		HN	64 GLY	HN	5.44697
	HB2	62 VAL	HN	4 30230		HA1	64 GLY	HN	3.566320
	HB2	111 VAL	HA	6 8607		HA1	111 VAL	HA	3.439040
	HB2	114 GLY	HN	6 7280		HA1	111 VAL	QG1	7 668
	HB3	61 ARG	HG2	3.379280		HA1	112 ALA	HN	3.344390
	HB3	61 ARG	HG3	4.315180		HA2	64 GLY	HN	4.125720
	HB3	61 ARG	QD	5.1 21265.0*2		HA2	111 VAL	HA	4.210530
	HB3	62 VAL	HN	4.220160		HA2	111 VAL	QG1	7 2091
	HB3	111 VAL	HA	6 8840		HA2	112 ALA	HN	4.57122
	HB3	111 VAL	QG1	7 5174	64 GLY				
	HB3	111 VAL	QG2	7 4408		HN	64 GLY	HA1	4.125840
	HB3	113 GLN	HA	6 1338		HN	64 GLY	HA2	4.123480
	HG2	61 ARG	QD	5 23805.0*2		HN	65 MET	HN	6 0
	HG2	62 VAL	HN	6 12880		HN	84 VAL	QG2	7 3430
	HG2	113 GLN	HA	6 1462		HN	109 GLY	HA1	6 960
	HG2	113 GLN	HB2	6 2329		HN	110 ILE	HN	3.534740
	HG2	113 GLN	HB3	6 5174		HN	111 VAL	HA	3.628140
	HG2	113 GLN	HG2	6 4881		HA1	65 MET	HN	3.654630
	HG2	113 GLN	HG3	6 2224		HA2	65 MET	HN	3.482930
	HG3	61 ARG	QD	5.2 18550.0*2		HA2	84 VAL	QG2	5.812750
	HG3	62 VAL	HN	6 10200	65 MET				
	HG3	113 GLN	HA	6 1616		HN	65 MET	HA	4.317560
	HG3	113 GLN	HB2	6 7282		HN	65 MET	HB2	4 27520
	HG3	113 GLN	HG2	6 4226		HN	65 MET	HB3	4 30030
	HG3	113 GLN	HG3	6 11010		HN	65 MET	HG2	4.96858
	HG3	114 GLY	HN	6 2079		HN	65 MET	HG3	4.610010
	QD	62 VAL	HN	7 365.0*2		HN	65 MET	QE	4.811560
	QD	111 VAL	QG2	7.8		HN	66 VAL	HN	5.25708
5815.0*2						HN	84 VAL	QG1	7 3554
	QD	128 LEU	QD1	8		HN	84 VAL	QG2	6.76323
1988.0*2						HN	85 HIS	HN	3.723090
	QD	128 LEU	QD2	8		HN	85 HIS	HB2	6 4746
548.0*2						HN	86 ASP	HA	5.61938
62 VAL						HA	65 MET	HB2	5.54058

HA	65	MET	HG2	6	607		QG2	82	PHE	CG	9	4808.5*2
HA	65	MET	HG3	6	0		QG2	82	PHE	CZ	9	2853.5*2
HA	65	MET	QE	5.8	3686		QG2	84	VAL	QG1	8	2414
HA	66	VAL	HN	3.2	116300		QG2	104	PHE	CZ	9	
HA	66	VAL	QG2	7	2342	2172.0*2						
HA	109	GLY	HA1	2.9	100000		QG2	104	PHE	HZ	7	2695
HA	109	GLY	HA2	3.5	33500		QG2	106	GLU	HA	6.6	7017
HA	110	ILE	HN	3.5	30860		QG2	107	GLY	HN	7	2719
HB2	65	MET	HG2	3.5	52010		QG2	108	GLN	HN	6.9	5360
HB2	65	MET	HG3	3.3	71160		QG2	110	ILE	QG2	5.2	66720
HB2	65	MET	QE	5	8668	67 THR						
HB2	66	VAL	HN	4.7	10140	HN	67 THR	HA	4.6	11440		
HB3	65	MET	HG2	3.3	73960	HN	67 THR	HB	3.9	33710		
HB3	65	MET	HG3	4	24260	HN	67 THR	QG2	4.8	10940		
HB3	65	MET	QE	4	35920	HN	68 VAL	HN	4.4	16640		
HB3	66	VAL	HN	4.8	8804	HN	70 SER	HB3	6	2069		
HB3	109	GLY	HA1	6	1925	HN	70 SER	HG	6	9216		
HG2	65	MET	QE	5.3	6273	HN	83 ALA	HN	6	893		
HG2	66	VAL	HN	6	8283	HN	84 VAL	HN	6	1245		
HG3	65	MET	QE	5.7	4032	HN	84 VAL	HA	4	14410		
HG3	66	VAL	HN	6	1609	HN	84 VAL	QG1	7	4960		
QE	66	VAL	HN	6.6	6562	HA	67 THR	HB	3.3	97310		
66 VAL						HA	67 THR	QG2	4.2	25940		
HN	66	VAL	HA	4.2	22240	HA	68 VAL	HN	3.6	53160		
HN	66	VAL	HB	3.8	41400	HA	68 VAL	QG1	6.4	8162		
HN	66	VAL	QG1	5	8413	HA	68 VAL	QG2	6.6	6676		
HN	66	VAL	QG2	3.7	52870	HA	69 GLY	HN	5.4	9711		
HN	67	THR	HN	6	2335	HB	67 THR	QG2	3.5	74760		
HN	107	GLY	HN	5.5	2104	HB	68 VAL	HN	5	7311		
HN	108	GLN	HN	3.4	40060	HB	70 SER	HN	5.5	8625		
HN	109	GLY	HA1	3.4	35910	HB	70 SER	HB2	5.6	20680		
HN	109	GLY	HA2	4.5	7567	HB	70 SER	HB3	6	8089		
HN	110	ILE	HN	6	1222	HB	70 SER	HG	5.2	32390		
HN	110	ILE	QD1	7	900	HB	83 ALA	HN	6	3047		
HA	66	VAL	HB	4.6	11570	HB	83 ALA	QB	6.7	6347		
HA	66	VAL	QG1	4.5	15660	QG2	68 VAL	HN	5.6	15360		
HA	66	VAL	QG2	3.7	51810	QG2	68 VAL	HB	5.9	12160		
HA	67	THR	HN	3.2	119900	QG2	68 VAL	QG1	6.4	18060		
HA	84	VAL	HA	3.7	22800	QG2	69 GLY	HN	6.5	7396		
HA	84	VAL	QG1	5.7	13790	QG2	70 SER	HN	7	1731		
HA	84	VAL	QG2	5.7	13780	QG2	70 SER	HA	5.3	20650		
HA	85	HIS	HN	6	787	QG2	70 SER	HB2	4.6	42670		
HB	66	VAL	QG1	4	31900	QG2	70 SER	HB3	5.1	23770		
HB	66	VAL	QG2	3.6	61920	QG2	70 SER	HG	4.8	34250		
HB	67	THR	HN	6	0	68 VAL						
HB	84	VAL	QG1	6.6	6958	HN	68 VAL	HA	3.6	51990		
HB	108	GLN	HN	5.5	23000	HN	68 VAL	HB	3.9	30920		
QG1	67	THR	HN	5.2	22410	HN	68 VAL	QG1	3.4	108700		
QG1	70	SER	HG	7	2622	HN	68 VAL	QG2	4.8	10670		
QG1	82	PHE	CG	9	2056.5*2	HN	69 GLY	HN	3.2	102300		
QG1	82	PHE	CZ	9	1730.0*2	HN	70 SER	HN	5.6	7719		
QG1	82	PHE	HZ	7	2694	HN	70 SER	HB2	6	3329		
QG1	84	VAL	HA	7	2343	HN	70 SER	HG	6	873		
QG1	84	VAL	QG2	7.3	8339	HN	106 GLU	HB2	6	6581		
QG1	104	PHE	CZ	9		HN	106 GLU	HB3	6	12120		
279.0*2						HA	68 VAL	HB	4	30260		
QG1	106	GLU	HA	4.8	34080	HA	68 VAL	QG1	4.5	17100		
QG1	107	GLY	HN	7	4078	HA	68 VAL	QG2	3.9	38120		
QG1	108	GLN	HN	7	1989	HA	69 GLY	HN	3.7	41880		
QG1	110	ILE	HG1	5	28540	HA	70 SER	HN	4.7	21080		
QG1	110	ILE	QD1	5.8	33950	HA	106 GLU	HA	4.7	5390		
QG2	67	THR	HN	5.8	13470	HA	106 GLU	HB2	6	13190		

HA	106	GLU	HB3	5.815330
HA	107	GLY	HN	6 1099
HA	107	GLY	HA2	4 13590
HB	68	VAL	QG1	4.226550
HB	68	VAL	QG2	4 33820
HB	69	GLY	HN	4.513460
HB	107	GLY	HN	6 4107
QG1	69	GLY	HN	5 28350
QG1	107	GLY	HN	6.38566
QG1	107	GLY	HA1	7 2465
QG1	107	GLY	HA2	7 3959
QG2	69	GLY	HN	4.738220
QG2	70	SER	HN	6.76311
QG2	107	GLY	HA1	7 2052
69	GLY			
	HN	69	GLY	HA1 3.469550
	HN	69	GLY	HA2 3.566450
	HN	70	SER	HN 3.744490
	HN	70	SER	HB2 5.82932
	HN	70	SER	HG 6 634
	HN	71	MET	HN 6 4982
	HA1	70	SER	HN 4.123740
	HA1	71	MET	HN 6 2045
	HA2	70	SER	HN 4.513990
	HA2	71	MET	HN 6 1236
70	SER			
	HN	70	SER	HA 3.656860
	HN	70	SER	HB2 4.612000
	HN	70	SER	HB3 4 29880
	HN	70	SER	HG 3.739960
	HN	71	MET	HN 3.481680
	HN	71	MET	HB2 5.83012
	HN	83	ALA	HN 5.81562
	HN	83	ALA	QB 7 1566
	HA	70	SER	HB2 3.1132600
	HA	70	SER	HB3 3.565320
	HA	70	SER	HG 4.96922
	HA	71	MET	HN 4.123360
	HA	83	ALA	HN 5.71632
	HA	83	ALA	QB 7 4811
	HB2	70	SER	HG 3.831200
	HB2	71	MET	HN 5.35025
	HB2	83	ALA	HN 6 7980
	HB2	83	ALA	QB 7 3584
	HB2	93	LEU	QD2 6.66611
	HB3	70	SER	HG 3.368750
	HB3	83	ALA	HN 6 9578
	HB3	83	ALA	QB 7 1985
	HG	71	MET	HN 6 4871
	HG	82	PHE	HA 6 718
	HG	83	ALA	HN 5.619770
71	MET			
	HN	71	MET	HA 3.744820
	HN	71	MET	HB2 3.931870
	HN	71	MET	HB3 4.123780
	HN	71	MET	HG2 4.96982
	HN	71	MET	HG3 4.87286
	HN	71	MET	QE 5.64550
	HN	72	VAL	HN 4.88804
	HN	72	VAL	QG2 7 1218
	HA	71	MET	HB2 4.124340
	HA	71	MET	HB3 4 28450

HA	71	MET	HG2	4.314790
HA	71	MET	HG3	4.216320
HA	71	MET	QE	5 9099
HA	72	VAL	HN	3 164100
HA	72	VAL	QG2	6.57302
HA	82	PHE	HA	3.349930
HA	82	PHE	HB2	5.913960
HA	82	PHE	HB3	4.946570
HA	83	ALA	HN	5 3626
HB2	71	MET	HG2	4.217390
HB2	71	MET	HG3	3.376680
HB2	71	MET	QE	4.418700
HB2	72	VAL	HN	5.16495
HB2	82	PHE	HB3	6 650
HB3	71	MET	HG2	3 122200
HB3	71	MET	HG3	3.299510
HB3	71	MET	QE	4.418110
HB3	72	VAL	HN	5.54176
HB3	82	PHE	HB2	6 10330
HG2	71	MET	QE	6 2964
HG2	72	VAL	HN	6 9650
HG2	80	VAL	QG1	7 3487
HG2	80	VAL	QG2	7 2111
HG2	82	PHE	HB2	6 8595
HG2	82	PHE	HB3	6 8399
HG2	106	GLU	HB3	6 13300
HG2	106	GLU	HG2	5.717360
HG2	106	GLU	HG3	5.619160
HG3	71	MET	QE	4.615340
HG3	72	VAL	HN	6 10320
HG3	80	VAL	QG1	7 4106
HG3	82	PHE	HB2	6 1891
HG3	82	PHE	HB3	6 12990
HG3	104	PHE	CZ	8
735.5*2				
	QE	72	VAL	HN 7 4262
	QE	80	VAL	HB 4.929440
	QE	82	PHE	HA 7 1680
	QE	82	PHE	HB3 6.95563
	QE	100	LEU	QD1 7.19756
	QE	100	LEU	QD2 7.57248
	QE	104	PHE	CZ 9
686.5*2				
72	VAL			
	HN	72	VAL	HA 3.838800
	HN	72	VAL	HB 4.513050
	HN	72	VAL	QG1 4.713330
	HN	72	VAL	QG2 4.418920
	HN	73	ARG	HN 4.611510
	HN	80	VAL	QG1 6.76456
	HN	81	GLN	HN 3.258080
	HN	81	GLN	HG2 6 685
	HN	81	GLN	HG3 6 4414
	HN	82	PHE	HA 3.531530
	HN	82	PHE	HB2 6 807
	HN	82	PHE	HB3 6 9069
	HA	72	VAL	HB 4.318790
	HA	72	VAL	QG1 4.517110
	HA	72	VAL	QG2 4.712480
	HA	73	ARG	HN 3 171400
	HB	72	VAL	QG1 4.614560
	HB	72	VAL	QG2 4.910370

HB	73	ARG	HN	5.2	5831	HN	79	HIS	HN	3.7	24570
HB	81	GLN	HN	6	6146	HN	80	VAL	HA	3.6	28210
HB	81	GLN	HG2	6	11680	HN	80	VAL	HB	6	637
HB	81	GLN	HE21	6	4029	HN	80	VAL	QG1	6.4	8022
HB	81	GLN	HE22	6	2403	HN	80	VAL	QG2	6.7	6369
QG1	73	ARG	HN	5.6	16170	HA	74	ASP	HB2	4.5	13780
QG1	81	GLN	HN	6.5	7426	HA	74	ASP	HB3	4.3	19170
QG1	81	GLN	HG2	7	4215	HA	75	PRO	HG3	6	2354
QG1	81	GLN	HE21	7	4192	HA	75	PRO	HD2	4.3	102200
QG1	81	GLN	HE22	6.8	5696	HA	75	PRO	HD3	4.6	68350
QG1	82	PHE	HA	7	2736	HA	76	ASN	HN	5.7	6851
QG1	82	PHE	CG	9	2275.0*2	HA	76	ASN	HD22	6	3285
QG2	73	ARG	HN	7	4556	HB2	76	ASN	HN	6	3040
QG2	81	GLN	HN	7	3141	HB2	76	ASN	HD22	6	3472
QG2	81	GLN	HB3	5.5	17450	HB2	79	HIS	HN	5.9	14660
QG2	81	GLN	HG2	7	2606	HB2	79	HIS	HB2	5.3	28500
QG2	81	GLN	HE21	7	5089	HB2	79	HIS	HB3	5.4	24940
QG2	81	GLN	HE22	6.7	6341	HB3	76	ASN	HD22	6	2312
73 ARG			HB3	78	LEU	HB3	78	LEU	HN	6	2980
HN	73	ARG	HA	3.6	50270	HB3	79	HIS	HN	6	2059
HN	73	ARG	HB2	4.1	23370	HB3	79	HIS	HB2	6	5744
HN	73	ARG	HB3	3.8	41420	HB3	79	HIS	HB3	5.8	16040
HN	73	ARG	QG	5.9	7175.0*2	HB3	79	HIS	HD2	6	855
HN	73	ARG	QD	5.9	6725.0*2	75 PRO					
HN	74	ASP	HN	5.8	3020	HA	75	PRO	HB2	3.3	85800
HA	73	ARG	HB2	4.1	26060	HA	75	PRO	HB3	3.8	41100
HA	73	ARG	HB3	4.3	18230	HA	75	PRO	HG2	4	22100
HA	73	ARG	QG	4.6	22820.0*2	HA	75	PRO	HG3	4.2	17550
HA	73	ARG	QD	6	6410.0*2	HA	75	PRO	HD2	5.5	3436
HA	74	ASP	HN	3.1	146400	HA	75	PRO	HD3	5.6	3164
HA	80	VAL	HA	3.1	67480	HA	76	ASN	HN	3.9	31660
HA	80	VAL	HB	6	3311	HA	77	SER	HN	5.7	6641
HA	80	VAL	QG2	5.4	18660	HA	78	LEU	QD1	7	436
HA	81	GLN	HN	3.3	50120	HB2	75	PRO	HG2	3.8	30980
HB2	73	ARG	QG	5.7	8480.0*2	HB2	75	PRO	HG3	3.8	31840
HB2	73	ARG	QD	5	21835.0*2	HB2	75	PRO	HD2	6	1790
HB2	74	ASP	HN	4.1	24240	HB2	75	PRO	HD3	5.2	4652
HB2	80	VAL	HA	6	5806	HB2	76	ASN	HN	5.7	3259
HB2	80	VAL	HB	4.8	53760	HB3	75	PRO	HG2	3.1	116400
HB2	80	VAL	QG1	5.7	13620	HB3	75	PRO	HG3	3.1	116500
HB2	80	VAL	QG2	5.6	15930	HB3	75	PRO	HD2	4.6	10050
HB3	73	ARG	QG	5.8	7965.0*2	HB3	75	PRO	HD3	4.3	14870
HB3	73	ARG	QD	4.9	26365.0*2	HB3	76	ASN	HN	5.2	5557
HB3	74	ASP	HN	4.3	18560	HG2	75	PRO	HD2	3.9	27520
HB3	80	VAL	QG1	5.7	14010	HG2	75	PRO	HD3	3.9	26100
HB3	80	VAL	QG2	5.9	12270	HG2	76	ASN	HN	6	3590
QG	73	ARG	QD	6.2	16265.0*4	HG2	76	ASN	HA	6	366
QG	74	ASP	HN	7	5170.0*2	HG2	76	ASN	HD22	6	2755
QG	80	VAL	HB	7	4477.5*2	HG3	75	PRO	HD2	4.1	20970
QG	80	VAL	QG2	8	4459.5*2	HG3	75	PRO	HD3	4.1	19410
QD	74	ASP	HN	7	5950.0*2	HG3	76	ASN	HN	6	5126
QD	80	VAL	HB	7	2393.0*2	HD2	76	ASN	HN	6	12500
QD	80	VAL	QG1	8	5060.0*2	HD2	78	LEU	QD1	7	1126
QD	80	VAL	QG2	8	2663.0*2	HD3	76	ASN	HN	6	8614
74 ASP			76 ASN								
HN	74	ASP	HA	3.6	52820	HN	76	ASN	HA	3.6	53130
HN	74	ASP	HB2	3.6	53900	HN	76	ASN	HB2	3.7	47100
HN	74	ASP	HB3	3.4	71150	HN	76	ASN	HB3	4.1	24440
HN	76	ASN	HN	6	2275	HN	76	ASN	HD21	5.8	2533
HN	76	ASN	HD22	6	609	HN	77	SER	HN	3.3	84980
HN	77	SER	HN	6	1478	HN	77	SER	HA	5	7037
HN	78	LEU	HN	6	1173	HN	78	LEU	HN	5.3	10900

HA	76 ASN	HB2	4.318290	HB3	78 LEU	HG	4.316020
HA	76 ASN	HB3	3.743340	HB3	78 LEU	QD1	4.99420
HA	76 ASN	HD21	5.43590	HB3	78 LEU	QD2	4.225060
HA	77 SER	HN	4.220880	HB3	79 HIS	HN	4.710360
HA	78 LEU	QD2	6.76275	HB3	98 ASP	HN	6 819
HB2	76 ASN	HD21	3.643390	HB3	98 ASP	HA	6 2897
HB2	76 ASN	HD22	4 23020	HB3	99 LEU	HN	6 1426
HB2	77 SER	HN	4.416490	HG	78 LEU	QD1	4.811660
HB2	78 LEU	HN	6 2155	HG	78 LEU	QD2	4.130490
HB2	79 HIS	HN	5.58472	HG	79 HIS	HN	6 5302
HB2	79 HIS	HB2	6 12390	QD1	79 HIS	HN	7 2735
HB2	79 HIS	HB3	5.815700	QD2	79 HIS	HN	7 4828
HB3	76 ASN	HD21	4.121110	QD2	98 ASP	HA	6.76129
HB3	76 ASN	HD22	4.88197	QD2	99 LEU	HN	5.911940
HB3	77 SER	HN	4.124130	79 HIS			
HB3	78 LEU	HN	6 1140	HN	79 HIS	HA	3.650750
HB3	79 HIS	HN	6 3093	HN	79 HIS	HB2	3.564910
77 SER				HN	79 HIS	HB3	3.748370
HN	77 SER	HA	3.742940	HN	80 VAL	HN	5.63567
HN	77 SER	HB2	4.221460	HA	79 HIS	HB2	3.930760
HN	77 SER	HB3	4.710990	HA	79 HIS	HB3	4.318150
HN	78 LEU	HN	3.838730	HA	80 VAL	HN	3.388030
HN	78 LEU	QD1	7 3394	HA	97 ASP	HA	3.258300
HN	78 LEU	QD2	7 2310	HA	97 ASP	HB2	6 1265
HN	79 HIS	HN	5.85929	HA	97 ASP	HB3	6 2298
HN	79 HIS	HD2	6 1840	HA	98 ASP	HN	5.23115
HA	77 SER	HB2	3.653110	HB2	79 HIS	HD2	6 1919
HA	77 SER	HB3	3.567090	HB2	80 VAL	HN	5.82955
HA	78 LEU	HN	3.654550	HB2	97 ASP	HB2	6 1441
HA	78 LEU	QD1	5.912250	HB3	79 HIS	HD2	5.92112
HA	79 HIS	HN	5.310590	HB3	80 VAL	HN	4.89471
HA	99 LEU	QD2	6.38749	HB3	97 ASP	HB2	6 10130
HB2	78 LEU	HN	4.611720	HD2	97 ASP	HB2	6 2719
HB2	78 LEU	QD1	7 1418	80 VAL			
HB2	99 LEU	QD2	7 795	HN	80 VAL	HA	3.932370
HB3	78 LEU	HN	4.611570	HN	80 VAL	HB	4.98416
HB3	99 LEU	QD1	6.57157	HN	80 VAL	QG1	4.615460
HB3	99 LEU	QD2	6.29336	HN	80 VAL	QG2	4.516880
78 LEU				HN	81 GLN	HN	5.25478
HN	78 LEU	HA	4.319270	HN	96 TYR	HN	3.437830
HN	78 LEU	HB2	4.125120	HN	97 ASP	HA	3.441110
HN	78 LEU	HB3	4.98237	HN	98 ASP	HN	6 822
HN	78 LEU	HG	4.97214	HA	80 VAL	HB	3.473130
HN	78 LEU	QD1	5.45606	HA	80 VAL	QG1	4.516420
HN	78 LEU	QD2	5.36168	HA	80 VAL	QG2	5.36166
HN	79 HIS	HN	3.841520	HA	81 GLN	HN	3 159500
HN	80 VAL	QG2	6.57271	HB	80 VAL	QG1	3.942070
HA	78 LEU	HB2	3.933190	HB	80 VAL	QG2	3.490220
HA	78 LEU	HB3	3.651830	HB	81 GLN	HN	3.836380
HA	78 LEU	HG	4.88225	QG1	81 GLN	HN	5.418590
HA	78 LEU	QD1	5.27199	QG1	82 PHE	CZ	9 974.0*2
HA	78 LEU	QD2	4 33930	QG1	96 TYR	HN	7 4931
HA	79 HIS	HN	4.123850	QG1	96 TYR	HB2	6.76110
HA	98 ASP	HA	3.626140	QG1	96 TYR	HB3	7 3361
HA	99 LEU	HG	6 3789	QG1	96 TYR	CG	9 2337.0*2
HA	99 LEU	QD1	7 1103	QG1	99 LEU	HA	7 1381
HA	99 LEU	QD2	7 2916	QG1	99 LEU	QD1	7.38691
HB2	78 LEU	HG	3.646450	QG1	99 LEU	QD2	6.517260
HB2	78 LEU	QD1	4.322560	QG1	100 LEU	HN	7 3056
HB2	78 LEU	QD2	4.223770	QG1	100 LEU	HB2	6.76170
HB2	79 HIS	HN	4.513930	QG1	100 LEU	HG	6.47714
HB2	98 ASP	HA	6 2197	QG1	100 LEU	QD1	7.29169

QG1	100	LEU	QD2	7.6	6845	HN	82	PHE	CZ	7	812.0*2
QG2	81	GLN	HN	6.9	5321	HN	83	ALA	HN	4.8	9906
QG2	82	PHE	CG	9	720.5*2	HN	93	LEU	QD2	5.1	25590
QG2	82	PHE	CZ	9	874.0*2	HN	94	VAL	HN	3.2	53700
QG2	96	TYR	HN	5.9	11700	HN	94	VAL	HB	6	11540
QG2	96	TYR	HB2	6.7	6108	HN	94	VAL	QG1	6.7	6494
QG2	96	TYR	HB3	7	4413	HN	94	VAL	QG2	6.5	7554
QG2	96	TYR	CG	9	1618.5*2	HN	95	THR	HA	3.6	29430
QG2	98	ASP	HN	7	894	HA	82	PHE	HB2	3.6	56410
QG2	99	LEU	HG	6.4	8074	HA	82	PHE	HB3	3.5	65120
QG2	100	LEU	HB2	5.6	15530	HA	82	PHE	CG	7	1822.0*2
QG2	100	LEU	QD1	7.3	8657	HA	83	ALA	HN	3.5	63770
QG2	100	LEU	QD2	7.5	7533	HB2	82	PHE	CG	7	6160.0*2
81	GLN					HB2	82	PHE	CZ	8	703.5*2
HN	81	GLN	HA	4.2	20840	HB2	83	ALA	HN	3.8	41500
HN	81	GLN	HB2	4.2	20350	HB3	82	PHE	CG	6.4	13730.0*2
HN	81	GLN	HB3	4.2	22080	HB3	82	PHE	CZ	8	169.5*2
HN	81	GLN	HG3	5.1	5177	HB3	82	PHE	HZ	6	1227
HN	81	GLN	HE21	6	1534	HB3	83	ALA	HN	4.1	23460
HN	81	GLN	HE22	6	1309	HB3	96	TYR	CG	8	1218.5*2
HA	81	GLN	HB2	4.1	23400	CG	82	PHE	CZ	7.8	30650.0*4
HA	81	GLN	HB3	4	27770	CG	82	PHE	HZ	5.1	119000.0*2
HA	81	GLN	HG2	3.7	37680	CG	83	ALA	HN	8	3695.5*2
HA	81	GLN	HG3	3.9	26770	CG	84	VAL	QG1	8	10885.0*2
HA	82	PHE	HN	3.1	128100	CG	84	VAL	QG2	9	1129.0*2
HA	82	PHE	CG	8	217.5*2	CG	94	VAL	QG1	9	1159.5*2
HA	95	THR	HA	3.1	65570	CG	94	VAL	QG2	9	1486.5*2
HA	95	THR	HB	6	4104	CG	100	LEU	QD1	9	
HA	95	THR	QG2	5.2	22390	326.5*2					
HA	96	TYR	HN	3.3	44170	CG	100	LEU	QD2	9	
HB2	81	GLN	HG2	3.7	37540	294.0*2					
HB2	81	GLN	HG3	3.5	49880	CG	104	PHE	CZ	10	
HB2	81	GLN	HE22	5.1	5472	107.3*4					
HB2	82	PHE	HN	4.4	15310	CZ	82	PHE	HZ	6.1	19705.0*2
HB2	93	LEU	QD1	7	3678	CZ	84	VAL	QG1	8	11140.0*2
HB2	95	THR	HA	6	1195	CZ	84	VAL	QG2	9	3285.0*2
HB2	95	THR	QG2	5.8	12890	CZ	94	VAL	HB	8	3136.5*2
HB2	96	TYR	HN	6	7259	CZ	94	VAL	QG1	9	4702.0*2
HB3	81	GLN	HG2	3	129000	CZ	94	VAL	QG2	9	2565.0*2
HB3	81	GLN	HG3	4.6	10080	CZ	96	TYR	CG	10	980.3*4
HB3	81	GLN	HE21	5.1	5213	CZ	96	TYR	CZ	10	198.3*4
HB3	81	GLN	HE22	6	1920	CZ	100	LEU	QD2	8.7	
HB3	82	PHE	HN	4.9	8316	6210.0*2					
HB3	95	THR	HA	6	859	CZ	104	PHE	CG	9.1	
HB3	96	TYR	HN	6	3508	35850.0*4					
HG2	81	GLN	HE21	3.5	49360	CZ	104	PHE	CZ	10	
HG2	81	GLN	HE22	4.1	19980	1358.5*4					
HG2	82	PHE	HN	6	8878	CZ	110	ILE	HB	8	
HG2	95	THR	QG2	6	10670	645.5*2					
HG3	81	GLN	HE21	4.1	19550	CZ	110	ILE	QG2	9	
HG3	81	GLN	HE22	5.5	3300	2153.5*2					
HG3	82	PHE	HN	5.8	15310	CZ	110	ILE	HG1	8	
HG3	95	THR	QG2	6.1	10220	422.0*2					
HE21	93	LEU	QD1	5.6	15900	5880.0*2					
HE21	93	LEU	QD2	5.8	13440	CZ	110	ILE	QD1	8.8	
HE22	93	LEU	QD1	5.7	13590	3730.0*2					
HE22	93	LEU	QD2	6	10810	HZ	84	VAL	QG1	6.3	8583
82	PHE					HZ	100	LEU	QD1	7	1333
HN	82	PHE	HA	3.6	50260	HZ	100	LEU	QD2	7	2538
HN	82	PHE	HB2	5.7	3371	HZ	104	PHE	CG	6.8	
HN	82	PHE	HB3	5.8	2862	48140.0*2					
HN	82	PHE	CG	8	2057.5*2						

HZ	104	PHE	CZ	8	
7320.0*2					
HZ	110	ILE	HB	6	1373
HZ	110	ILE	HG1	6	989
HZ	110	ILE	QD1	6.7	6345
HZ	127	VAL	QG1	7	2552
HZ	127	VAL	QG2	7	2730

83 ALA					
HN	83	ALA	HA	4	28290
HN	83	ALA	QB	3.5	32990
HA	83	ALA	QB	3.4	102900
HA	84	VAL	HN	3.4	74760
HA	92	ILE	QG2	6.5	7262
HA	93	LEU	HA	3.1	71030
HA	93	LEU	QD1	7	2530
HA	93	LEU	QD2	5	26420
HA	94	VAL	HN	3.2	59660
QB	84	VAL	HN	4	13970
QB	91	GLU	HG2	6.2	9199
QB	91	GLU	HG3	6.2	9288
QB	92	ILE	HN	7	3881
QB	93	LEU	HN	6.3	8480
QB	93	LEU	HA	6.2	9594
QB	93	LEU	HG	4.4	52660
QB	93	LEU	QD1	6.2	23590
QB	93	LEU	QD2	6.8	12630
QB	94	VAL	HN	6.2	8920

84 VAL					
HN	84	VAL	HA	4.1	23250
HN	84	VAL	HB	3.9	31760
HN	84	VAL	QG1	4.4	19370
HN	84	VAL	QG2	5.2	7293
HN	85	HIS	HN	4.5	14030
HN	85	HIS	HD2	6	8906
HN	92	ILE	HN	3.2	59680
HN	92	ILE	QG2	6	10520
HN	92	ILE	QD1	7	2471
HN	93	LEU	HA	3.4	41360
HN	93	LEU	QD2	5.7	14080
HA	84	VAL	HB	4.5	14720
HA	84	VAL	QG1	4.7	13510
HA	84	VAL	QG2	3.9	42770
HA	85	HIS	HN	3.1	133000
HA	92	ILE	QG2	7	1393
HB	84	VAL	QG1	4	35640
HB	84	VAL	QG2	3.6	61220
HB	85	HIS	HN	5.2	6052
HB	92	ILE	QG2	6	11420
HB	94	VAL	QG1	7	4528
HB	94	VAL	QG2	7	4652
QG1	85	HIS	HN	5.8	12710
QG1	92	ILE	HN	7	1082
QG1	92	ILE	QG2	7	10680
QG1	94	VAL	HB	5.7	14270
QG1	94	VAL	QG1	7.9	5471
QG1	94	VAL	QG2	6.5	16610
QG1	104	PHE	CZ	9	
319.5*2					
QG2	85	HIS	HN	5.1	25850
QG2	92	ILE	HB	7	4901
QG2	92	ILE	QG1	8	1466.0*2
QG2	109	GLY	HA2	7	3686

85 HIS					
HN	85	HIS	HA	4.5	13840
HN	85	HIS	HB2	6	1956
HN	85	HIS	HB3	5.8	3120
HN	85	HIS	HD2	6	957
HN	86	ASP	HN	4.5	13930
HA	85	HIS	HB2	3.8	40880
HA	85	HIS	HB3	4.1	22670
HA	86	ASP	HN	3.4	82120
HA	91	GLU	HA	3.1	68140
HA	91	GLU	QB	7	4172.0*2
HA	91	GLU	HG2	6	1742
HA	91	GLU	HG3	6	2352
HA	92	ILE	HN	4.1	13270
HB2	85	HIS	HD2	4.1	19030
HB2	85	HIS	HE1	6	1363
HB2	86	ASP	HN	4	29430
HB2	86	ASP	HB3	6	9237
HB2	91	GLU	QB	7	1272.0*2
HB2	91	GLU	HG3	6	12430
HB3	85	HIS	HD2	4.8	8154
HB3	85	HIS	HE1	5.5	3539
HB3	86	ASP	HN	4.7	11140
HB3	91	GLU	HA	6	1546
HB3	91	GLU	QB	7	506.0*2
HB3	91	GLU	HG2	6	3315
HD2	86	ASP	HA	6	2266
HD2	91	GLU	HA	6	2534

86 ASP					
HN	86	ASP	HA	4.5	14240
HN	86	ASP	HB2	4.1	24850
HN	86	ASP	HB3	4.8	9445
HN	88	LEU	HN	4.7	22800
HN	90	GLY	HN	4.3	37430
HN	91	GLU	HA	4.6	6036
HN	91	GLU	HG2	6	1032
HA	86	ASP	HB2	3.7	42660
HA	86	ASP	HB3	3.8	39400
HA	88	LEU	HN	6	573
HB2	88	LEU	HN	6	4028
HB3	88	LEU	HN	6	440

88 LEU					
HN	88	LEU	HA	3.7	43000
HN	88	LEU	HB2	3.5	61840
HN	88	LEU	HB3	4.1	25140
HN	88	LEU	HG	4.4	13020
HN	88	LEU	QD1	5.9	3145
HN	88	LEU	QD2	6.1	2534
HN	89	GLY	HN	3.7	45090
HN	89	GLY	HA2	6	1958
HN	90	GLY	HN	5.4	9037
HN	90	GLY	HA1	6	1586
HA	88	LEU	HB2	4.2	22130
HA	88	LEU	HB3	3.5	62190
HA	88	LEU	HG	5.7	2827
HA	88	LEU	QD1	5	8952
HA	88	LEU	QD2	4.2	23970
HA	89	GLY	HN	3.6	50430
HB2	88	LEU	HG	3.3	73140
HB2	88	LEU	QD1	5.4	5258
HB2	88	LEU	QD2	5.1	7712
HB2	89	GLY	HN	5.1	6176

HB2	90 GLY	HN	5.49018		QG1	122 LEU	QD1 8
HB3	88 LEU	HG	4.314710	4408.0*2			
HB3	88 LEU	QD1	4.810620		QG1	122 LEU	QD2 8
HB3	88 LEU	QD2	4.712640	2667.5*2			
HB3	89 GLY	HN	4.89356		QD1	93 LEU	HN 5.714210
HB3	90 GLY	HN	5.310790		QD1	121 LYS	HD2 5.418440
HG	88 LEU	QD1	4.615270		QD1	122 LEU	HN 5.912400
HG	88 LEU	QD2	4.615460		QD1	122 LEU	HB2 6.48095
HG	89 GLY	HN	6 4468		QD1	122 LEU	QD2 5.835280
89 GLY				93 LEU			
HN	89 GLY	HA1	4.125720		HN	93 LEU	HA 4.220530
HN	89 GLY	HA2	3.933040		HN	93 LEU	HB2 3.563890
HN	90 GLY	HN	3.558920		HN	93 LEU	HB3 4.122690
HN	90 GLY	HA2	6 707		HN	93 LEU	HG 4.87567
HA1	90 GLY	HN	6 632		HN	93 LEU	QD1 5.45262
HA2	90 GLY	HN	5.25869		HN	93 LEU	QD2 5.73777
90 GLY					HN	94 VAL	HN 5.54084
HN	90 GLY	HA1	4 27940		HN	121 LYS	QG 7
HN	90 GLY	HA2	3.653240	6220.0*2			
HN	91 GLU	HN	5 7002		HN	121 LYS	HD2 5.232340
HA1	91 GLU	HN	3.478020		HN	122 LEU	HN 5.71787
HA2	91 GLU	HN	3.747600		HN	122 LEU	HG 6 4152
91 GLU					HA	93 LEU	HB2 3.838300
HN	91 GLU	HA	4.124890		HA	93 LEU	HB3 3.567720
HN	91 GLU	QB	4.3 45335.0*2		HA	93 LEU	HG 5.34481
HN	91 GLU	HG2	6 1835		HA	93 LEU	QD1 4.810890
HN	91 GLU	HG3	6 1943		HA	93 LEU	QD2 4.99589
HN	92 ILE	HN	6 1834		HA	94 VAL	HN 3.478260
HA	91 GLU	QB	4.8 37060.0*2		HB2	93 LEU	HG 3.458620
HA	91 GLU	HG2	3.927010		HB2	93 LEU	QD1 6.22322
HA	91 GLU	HG3	3.926970		HB2	93 LEU	QD2 5.55118
HA	92 ILE	HN	3.2113700		HB2	94 VAL	HN 4.710440
HA	92 ILE	QG2	7 1193		HB2	95 THR	QG2 7 1514
QB	91 GLU	HG2	4.6 45375.0*2		HB2	121 LYS	HB3 5.327310
QB	91 GLU	HG3	5.5 11220.0*2		HB2	121 LYS	HD3 5.521950
QB	92 ILE	HN	6.1 6735.0*2		HB2	121 LYS	HE2 6 3387
HG2	92 ILE	HN	5.619100		HB3	93 LEU	HG 3.1113500
HG3	92 ILE	HN	5.521910		HB3	93 LEU	QD1 4.420050
92 ILE					HB3	93 LEU	QD2 4.811160
HN	92 ILE	HA	4 30440		HB3	94 VAL	HN 4.220840
HN	92 ILE	HB	4.611370		HB3	121 LYS	HB3 5.424080
HN	92 ILE	QG2	5 8714		HB3	121 LYS	QG 7
HN	92 ILE	QG1	5.9 6750.0*2	10380.0*2			
HN	92 ILE	QD1	5.64359		HG	93 LEU	QD1 5.64376
HA	92 ILE	HB	4.611340		HG	93 LEU	QD2 4.615180
HA	92 ILE	QG2	5.26932		HG	94 VAL	HN 5.329230
HA	92 ILE	QG1	5.5 6865.0*2		QD1	94 VAL	HN 6.48135
HA	92 ILE	QD1	4.131070		QD1	121 LYS	QG 8
HA	93 LEU	HN	3.396890	4231.5*2			
HB	92 ILE	QG2	4.418660		QD1	121 LYS	HE2 7 4498
HB	92 ILE	QG1	7 1229.5*2		QD1	121 LYS	HE3 7 4337
HB	92 ILE	QD1	4.225560		QD2	94 VAL	HN 4.449710
HB	93 LEU	HN	4.414900		QD2	121 LYS	QG 7.6
QG2	92 ILE	QG1	5.7 12170.0*2	6540.0*2			
QG2	92 ILE	QD1	4.752060		QD2	121 LYS	HE2 7 4709
QG2	93 LEU	HN	7 3261		QD2	121 LYS	HE3 7 4306
QG2	94 VAL	QG1	6.813220	94 VAL			
QG2	122 LEU	QD2	5.263320		HN	94 VAL	HA 4 29840
QG1	92 ILE	QD1	4.6 65800.0*2		HN	94 VAL	HB 4 26230
QG1	93 LEU	HN	7 10005.0*2		HN	94 VAL	QG1 5.17987
QG1	121 LYS	HD2	7		HN	94 VAL	QG2 4.226270
7360.0*2					HN	95 THR	HN 5.16769

HA	94 VAL	HB	4.220410
HA	94 VAL	QG1	4 32770
HA	94 VAL	QG2	3.937710
HA	95 THR	HN	3.388900
HA	95 THR	QG2	4.735930
HA	122 LEU	HN	3.819620
HA	122 LEU	HB2	6 10380
HA	122 LEU	HB3	6 907
HB	94 VAL	QG1	3.486140
HB	94 VAL	QG2	4.322120
HB	95 THR	HN	5.35128
HB	124 ALA	QB	6.95468
QG1	95 THR	HN	4.929720
QG1	95 THR	HA	7 1060
QG1	104 PHE	CG	9
1073.5*2			
QG1	112 ALA	QB	5.930870
QG1	121 LYS	QG	8
2663.0*2			
QG1	122 LEU	HN	6.48227
QG1	122 LEU	HB2	5.516780
QG1	122 LEU	HB3	4.454980
QG1	122 LEU	QD2	6.616020
QG1	124 ALA	HN	5.125240
QG1	124 ALA	QB	7.48078
QG2	95 THR	HN	5.418060
QG2	112 ALA	QB	6.124400
QG2	121 LYS	QG	8
3579.0*2			
QG2	122 LEU	HN	6.66964
QG2	122 LEU	HB2	5.517050
QG2	124 ALA	HN	7 2345
QG2	124 ALA	QB	8 2116
95 THR			
HN	95 THR	HA	3.931530
HN	95 THR	HB	4.89663
HN	95 THR	QG2	4.322240
HN	96 TYR	HN	5 7453
HN	121 LYS	QG	7
707.5*2			
HN	122 LEU	HN	3.531700
HN	123 ALA	HA	3.168240
HN	124 ALA	HN	3.437130
HA	95 THR	HB	3.558700
HA	95 THR	QG2	3.575690
HA	96 TYR	HN	3.389620
HB	95 THR	QG2	3.4123000
HB	96 TYR	HN	4.317260
HB	123 ALA	HA	6 1017
HB	123 ALA	QB	7 3153
QG2	96 TYR	HN	5.517360
QG2	121 LYS	HB2	7 3811
QG2	123 ALA	HA	7 1001
96 TYR			
HN	96 TYR	HA	4.611490
HN	96 TYR	HB2	3.836030
HN	96 TYR	HB3	5.25977
HN	97 ASP	HN	5.54210
HA	96 TYR	HB2	4.710060
HA	96 TYR	HB3	4.317370
HA	96 TYR	CG	5.8 7550.0*2
HA	97 ASP	HN	3.1127900

HA	124 ALA	HN	4.39816
HB2	96 TYR	CG	6.6 9715.0*2
HB2	97 ASP	HN	5.73365
HB3	96 TYR	CG	7.2 4680.5*2
HB3	97 ASP	HN	4.97992
HB3	100 LEU	QD1	7 911
HB3	100 LEU	QD2	7 748
HB3	127 VAL	QG2	7 3737
CG	96 TYR	CZ	7.5 54525.0*4
CG	96 TYR	HH	6.5 11245.0*2
CG	97 ASP	HN	8 8580.0*2
CG	98 ASP	HN	8 1493.0*2
CG	100 LEU	QD2	8.5
7345.0*2			
CG	124 ALA	QB	8.4
7640.0*2			
CG	125 THR	HG1	8
5760.0*2			
CG	127 VAL	QG2	9
2145.0*2			
CZ	96 TYR	HH	5.2 89050.0*2
CZ	98 ASP	HN	8 6575.0*2
CZ	98 ASP	HB2	8 5175.0*2
CZ	98 ASP	HB3	8 2599.0*2
CZ	100 LEU	HA	8
6970.0*2			
CZ	100 LEU	QD1	9
4372.0*2			
CZ	100 LEU	QD2	9
4380.0*2			
CZ	125 THR	HA	8
411.5*2			
CZ	125 THR	HG1	6.8
48720.0*2			
CZ	126 GLU	HN	8
1056.0*2			
CZ	127 VAL	HN	8
2279.0*2			
CZ	127 VAL	QG2	8.6
6545.0*2			
HH	98 ASP	HB2	6 4314
HH	100 LEU	HA	6 1540
HH	100 LEU	QD2	7 5071
HH	125 THR	HA	6 1349
HH	125 THR	HG1	5.718030
HH	126 GLU	HA	6 3042
HH	127 VAL	HN	6 1793
HH	127 VAL	HB	6 803
HH	127 VAL	QG2	7 4331
97 ASP			
HN	97 ASP	HA	3.934280
HN	97 ASP	HB2	3.742620
HN	97 ASP	HB3	3.655990
HN	98 ASP	HN	3.838850
HA	97 ASP	HB2	4.415850
HA	97 ASP	HB3	4.318220
HA	98 ASP	HN	3.839000
HB2	98 ASP	HN	5 7332
HB3	98 ASP	HN	5.92578
98 ASP			
HN	98 ASP	HA	3.652770
HN	98 ASP	HB2	4 26870

	HN	98	ASP	HB3	4	29190		HA	127	VAL	QG2	6.95315
	HN	99	LEU	HN	5.9	2562		HB2	100	LEU	HG	4.314940
	HA	98	ASP	HB2	4.7	10010		HB2	100	LEU	QD1	4.712710
	HA	98	ASP	HB3	4.6	11380		HB2	100	LEU	QD2	5.55085
	HA	99	LEU	HN	3.3	85240		HB2	101	PRO	HD3	5.914040
	HA	99	LEU	HB2	6	2399		HB2	103	LEU	HA	4.151540
	HA	99	LEU	HB3	6	2403		HB3	100	LEU	HG	4.412840
	HA	99	LEU	QD2	7	3072		HB3	100	LEU	QD1	4.811190
	HB2	99	LEU	HN	4.5	14460		HB3	100	LEU	QD2	5 8685
	HB2	99	LEU	QD1	7	1500		HB3	101	PRO	HG3	5.232970
	HB2	125	THR	HG1	6	2084		HB3	101	PRO	HD2	6 1377
	HB3	99	LEU	HN	4.8	8866		HB3	101	PRO	HD3	4.758550
99	LEU							HB3	104	PHE	HN	6 491
	HN	99	LEU	HA	4	30070		HB3	104	PHE	HB2	6 1222
	HN	99	LEU	HB2	3.4	77000		HB3	127	VAL	HB	6 5375
	HN	99	LEU	HB3	4	27920		HB3	127	VAL	QG1	7 3834
	HN	99	LEU	HG	4.3	15070		HG	100	LEU	QD1	4 33080
	HN	99	LEU	QD1	5.7	3891		HG	100	LEU	QD2	3.939500
	HN	99	LEU	QD2	5.4	5310		QD1	101	PRO	HG3	7 277
	HN	100	LEU	HN	4.7	10880		QD1	101	PRO	HD2	7 1164
	HA	99	LEU	HB2	3.9	35020		QD1	101	PRO	HD3	6.66969
	HA	99	LEU	HB3	4	26520		QD1	104	PHE	HB2	7 842
	HA	99	LEU	HG	4.2	17780		QD1	104	PHE	HB3	7 1746
	HA	99	LEU	QD1	4.4	19850		QD1	104	PHE	CG	9
	HA	99	LEU	QD2	4.5	16100	881.5*2					
	HA	100	LEU	HN	3.3	99110	QD1	104	PHE	CZ	9	
	HA	100	LEU	HB2	4.6	12200	2102.0*2					
	HA	100	LEU	HG	6	1596	QD1	127	VAL	HB	6.38850	
	HA	100	LEU	QD1	7	1316	QD1	127	VAL	QG1	7.57385	
	HB2	99	LEU	HG	3.4	61800	QD2	101	PRO	HG2	7 1460	
	HB2	99	LEU	QD1	4.4	19470	QD2	101	PRO	HD2	5.517580	
	HB2	99	LEU	QD2	4.1	29000	QD2	101	PRO	HD3	5.222040	
	HB2	100	LEU	HN	4.1	23460	QD2	104	PHE	HB2	7 1036	
	HB3	99	LEU	HG	3.4	60260	QD2	104	PHE	HB3	7 677	
	HB3	99	LEU	QD1	4.5	16700	QD2	104	PHE	CG	9	
	HB3	99	LEU	QD2	4.3	22560	3866.0*2					
	HB3	100	LEU	HN	4.3	18830	QD2	104	PHE	CZ	9	
	HG	99	LEU	QD1	4.5	16540	907.0*2					
	HG	99	LEU	QD2	4.3	23230	QD2	125	THR	HG1	7 2073	
	HG	100	LEU	HN	6	11370	QD2	127	VAL	QG1	8 4834	
	QD1	100	LEU	HN	6.7	6122	QD2	127	VAL	QG2	7.38362	
	QD2	100	LEU	HN	7	3726	101	PRO				
100	LEU						HA	101	PRO	HB2	4.123670	
	HN	100	LEU	HA	4.2	22270	HA	101	PRO	HB3	3.474160	
	HN	100	LEU	HB2	3.6	54130	HA	101	PRO	HG2	4.314670	
	HN	100	LEU	HB3	4.8	9169	HA	101	PRO	HG3	6 1507	
	HN	100	LEU	HG	4.5	10940	HA	101	PRO	HD2	6 1146	
	HN	100	LEU	QD1	5.7	4050	HA	101	PRO	HD3	6 479	
	HN	100	LEU	QD2	5.2	7111	HA	102	ASP	HN	3.841370	
	HN	101	PRO	HD2	6	1770	HA	103	LEU	HN	5.95482	
	HN	101	PRO	HD3	6	964	HB2	101	PRO	HG2	3.645520	
	HN	103	LEU	HN	6	1614	HB2	101	PRO	HG3	3.739080	
	HA	103	LEU	HA	5.8	6403	HB2	101	PRO	HD2	5 6125	
	HA	100	LEU	HB2	3.7	43470	HB2	101	PRO	HD3	6 430	
	HA	100	LEU	HB3	4.1	23240	HB2	102	ASP	HN	4.88899	
	HA	100	LEU	HG	4.5	10920	HB2	103	LEU	HN	6 3483	
	HA	100	LEU	QD1	5.1	8210	HB2	104	PHE	HN	5.76795	
	HA	100	LEU	QD2	4.3	21350	HB3	101	PRO	HG2	3.737430	
	HA	101	PRO	HD2	4.5	77170	HB3	101	PRO	HG3	3.553640	
	HA	101	PRO	HD3	4.9	47350	HB3	101	PRO	HD2	6 858	
	HA	125	THR	HG1	6	994	HB3	101	PRO	HD3	6 531	
	HA	127	VAL	QG1	7	2306	HB3	102	ASP	HN	6 1271	

	HB3	103	LEU	HN	6	1509		HB2	103	LEU	QD1	3.845040
	HG2	101	PRO	HD2	4	22580		HB2	103	LEU	QD2	5.26770
	HG2	101	PRO	HD3	4.5	11350		HB3	103	LEU	HG	4 24800
	HG2	102	ASP	HN	6	7049		HB3	103	LEU	QD1	4 33450
	HG2	104	PHE	HN	6	849		HB3	103	LEU	QD2	6.41969
	HG2	110	ILE	QD1	7	3389		HB3	104	PHE	HN	4.711150
	HG2	127	VAL	QG1	7	1994		HG	103	LEU	QD1	5.26931
	HG2	127	VAL	QG2	7	1327		HG	103	LEU	QD2	5.83748
	HG2	129	ALA	QB	6.8	5944		HG	104	PHE	HN	6 13110
	HG3	101	PRO	HD2	4.7	8896		HG	105	ARG	HN	6 4560
	HG3	101	PRO	HD3	4.5	11260		HG	105	ARG	HA	6 2312
	HG3	102	ASP	HN	6	8775		HG	105	ARG	HB2	6 1204
	HG3	104	PHE	HN	6	1942		HG	105	ARG	HG3	6 4136
	HG3	110	ILE	QD1	7	4709		QD1	104	PHE	HN	7 4039
	HG3	127	VAL	HB	6	9043		QD1	105	ARG	HB3	7 4050
	HG3	127	VAL	QG1	7	1650		QD2	104	PHE	HN	6.57248
	HG3	129	ALA	QB	7	2949		QD2	104	PHE	CG	9
	HD2	102	ASP	HN	6	8582	1671.0*2					
	HD2	104	PHE	HN	6	556		QD2	105	ARG	HD2	6.57510
	HD2	127	VAL	HB	6	913						
	HD2	127	VAL	QG1	7	3376		HN	104	PHE	HA	3.655280
	HD2	127	VAL	QG2	7	1095		HN	104	PHE	HB2	4 26460
	HD3	104	PHE	HB3	6	1589		HN	104	PHE	HB3	3.835800
	HD3	104	PHE	CG	8			HN	104	PHE	CG	7.3
464.0*2							4151.5*2					
	HD3	127	VAL	QG1	6.5	7457		HN	105	ARG	HN	3.567660
	HD3	127	VAL	QG2	6.3	8675		HA	104	PHE	HB2	4.611740
102	ASP							HA	104	PHE	HB3	4.611550
	HN	102	ASP	HA	4.7	11310		HA	104	PHE	CG	7
	HN	102	ASP	HB2	6	2266	1240.5*2					
	HN	102	ASP	HB3	4.1	25260		HA	105	ARG	HN	3.654610
	HN	103	LEU	HN	4.1	25660		HA	110	ILE	QG2	7 4691
	HN	103	LEU	HB3	6	1733		HA	129	ALA	QB	7 2323
	HN	104	PHE	HN	6	1427		HB2	104	PHE	CG	6.8
	HA	102	ASP	HB3	3.2	101000	7270.0*2					
	HA	103	LEU	HN	4.3	17230		HB2	105	ARG	HN	6 1988
	HA	104	PHE	HN	5.1	13250		HB2	110	ILE	QG2	7 1586
	HA	105	ARG	HN	6	3890		HB2	127	VAL	QG1	7 1591
	HA	105	ARG	HG2	6	4633		HB3	104	PHE	CG	6.9
	HA	105	ARG	HD2	6	704	6995.0*2					
	HB3	103	LEU	HN	4.9	7881		HB3	105	ARG	HN	5.82867
	HB3	103	LEU	HB3	6	7759		CG	104	PHE	CZ	7.2
	HB3	103	LEU	QD1	6.3	8656	87275.0*4					
	HB3	104	PHE	HN	5.6	7305		CG	104	PHE	HZ	5.6
	HB3	105	ARG	HA	6	3749	43190.0*2					
	HB3	105	ARG	HD3	6	4714		CG	105	ARG	HN	8
103	LEU						1178.5*2					
	HN	103	LEU	HA	3.7	42160		CG	110	ILE	HG1	8
	HN	103	LEU	HB2	4.8	9537	560.5*2					
	HN	103	LEU	HB3	4.2	20640		CG	110	ILE	QD1	7.7
	HN	103	LEU	HG	5.7	2736	13700.0*2					
	HN	103	LEU	QD1	5.5	4777		CG	127	VAL	QG1	8.9
	HN	103	LEU	QD2	5.8	3471	5420.0*2					
	HN	104	PHE	HN	3.6	50710		CG	127	VAL	QG2	9
	HN	105	ARG	HN	6	3755	2068.5*2					
	HA	103	LEU	HB2	4.7	11190		CZ	104	PHE	HZ	6
	HA	103	LEU	HB3	3.7	45390	24865.0*2					
	HA	103	LEU	HG	4	25090		CZ	110	ILE	QG2	9
	HA	103	LEU	QD1	3.9	42790	1316.0*2					
	HA	104	PHE	HN	4.3	18430		CZ	110	ILE	HG1	8
	HA	105	ARG	HN	6	1494	613.5*2					
	HB2	103	LEU	HG	4.7	8363						

	CZ	110	ILE	QD1	9		HB3	107	GLY	HN	4.1	25020
1970.5*2							HG3	107	GLY	HN	5.9	13930
	CZ	127	VAL	QG1	9	107	GLY					
2093.5*2							HN	107	GLY	HA1	3.3	84030
	HZ	110	ILE	HG1	6 2199		HN	107	GLY	HA2	4	29430
105	ARG						HN	108	GLN	HN	3.7	46610
	HN	105	ARG	HA	4.1 23420		HA1	108	GLN	HN	4.4	16540
	HN	105	ARG	HB2	4.2 22190		HA2	108	GLN	HN	4.8	8851
	HN	105	ARG	HB3	4.3 18140	108	GLN					
	HN	105	ARG	HG2	4.5 11290		HN	108	GLN	HA	3.7	43140
	HN	105	ARG	HG3	4.4 12470		HN	108	GLN	HB2	3.9	31270
	HN	106	GLU	HN	6 1859		HN	108	GLN	HB3	4	29400
	HA	105	ARG	HB2	4.5 13990		HN	108	GLN	QG	5.5	
	HA	105	ARG	HB3	4.2 20610	11595.0*2						
	HA	105	ARG	HG2	4.5 11950		HN	108	GLN	HE2	4.6	9978
	HA	105	ARG	HG3	4.8 7280		HN	108	GLN	HE2	6	2022
	HA	105	ARG	HD2	4.9 6739		HN	109	GLY	HN	5.9	2670
	HA	105	ARG	HD3	6 535		HN	131	HIS	HB2	6	3008
	HA	106	GLU	HN	3.4 71560		HA	108	GLN	HB2	4	28230
	HB2	105	ARG	HG2	3.3 70650		HA	108	GLN	HB3	4.4	15440
	HB2	105	ARG	HG3	3.9 28460		HA	108	GLN	QG	6.2	
	HB2	105	ARG	HD2	4.5 11150	2977.0*2						
	HB2	105	ARG	HD3	4.6 9627		HA	109	GLY	HN	3.6	57520
	HB2	106	GLU	HN	4.7 10460		HB2	108	GLN	QG	5	
	HB3	105	ARG	HG2	4.2 17660	23915.0*2						
	HB3	105	ARG	HG3	3.7 40570		HB2	108	GLN	HE2	4.4	13880
	HB3	105	ARG	HD2	4.6 10290		HB2	108	GLN	HE2	5.6	3122
	HB3	105	ARG	HD3	4.2 17210		HB2	109	GLY	HN	3.9	30590
	HB3	106	GLU	HN	4.9 8624		HB3	108	GLN	QG	4.4	
	HB3	108	GLN	HN	6 3154	61850.0*2						
	HB3	108	GLN	QG	7		HB3	108	GLN	HE2	5.9	2304
2459.0*2							HB3	109	GLY	HN	4.5	13480
	HB3	108	GLN	HE2	6 1041		QG	108	GLN	HE2	5.7	
	HB3	108	GLN	HE2	6 721	9075.0*2						
	HG2	105	ARG	HD2	4.2 16720		QG	108	GLN	HE2	7	
	HG2	105	ARG	HD3	4.1 20160	1884.0*2						
	HG2	106	GLU	HN	6 12490		QG	109	GLY	HN	7	
	HG2	108	GLN	HE2	6 983	3786.0*2						
	HG3	105	ARG	HD2	3.8 31400		QG	110	ILE	QD1	8	
	HG3	105	ARG	HD3	4.3 16140	1956.0*2						
	HG3	106	GLU	HN	6 10930		HE21	109	GLY	HN	6	583
	HG3	108	GLN	HE2	6 3390		HE22	129	ALA	QB	7	1381
	HG3	108	GLN	HE2	6 612	109	GLY					
106	GLU						HN	109	GLY	HA1	3.8	36500
	HN	106	GLU	HA	3.8 40910		HN	109	GLY	HA2	3.3	90180
	HN	106	GLU	HB2	4.3 19210		HN	110	ILE	HN	4.6	11460
	HN	106	GLU	HB3	3.9 33400		HA1	110	ILE	HN	3.5	66150
	HN	106	GLU	HG2	3.7 37480		HA1	110	ILE	QG2	7	3590
	HN	106	GLU	HG3	4.8 7956		HA2	110	ILE	HN	3.7	45270
	HN	107	GLY	HN	5.9 2699	110	ILE					
	HA	106	GLU	HB2	3.6 50200		HN	110	ILE	HA	4.4	15760
	HA	106	GLU	HB3	3.3 89090		HN	110	ILE	HB	5	7508
	HA	106	GLU	HG2	5.1 5380		HN	110	ILE	QG2	4.7	12770
	HA	106	GLU	HG3	4.6 10500		HN	110	ILE	HG1	3.9	27110
	HA	107	GLY	HN	3.3 93080		HN	110	ILE	HG1	4.5	11610
	HA	108	GLN	HN	5.3 10410		HN	110	ILE	QD1	5.4	5574
	HB2	106	GLU	HG2	3.8 31310		HN	111	VAL	HN	5.5	4210
	HB2	106	GLU	HG3	4.8 7483		HA	110	ILE	HB	3.4	72710
	HB2	107	GLY	HN	4.6 11900		HA	110	ILE	QG2	3.7	54620
	HB2	108	GLN	HN	6 1572		HA	110	ILE	HG1	4.3	15580
	HB3	106	GLU	HG2	3.6 46150		HA	110	ILE	HG1	4.7	8782
	HB3	106	GLU	HG3	4.7 8645		HA	110	ILE	QD1	4.7	12360

HA	111	VAL	HN	3.391270					
HA	127	VAL	HB	6 1648	15655.0*2				
HA	128	LEU	HN	6 833	QG2	130	LYS	QD	6.6
HA	129	ALA	HA	3.441540	1499.5*2				
HA	129	ALA	QB	7 1350	112	ALA			
HA	130	LYS	HN	4.211220	HN	112	ALA	HA	4 27670
HB	110	ILE	QG2	4.320580	HN	112	ALA	QB	3.456410
HB	110	ILE	HG1	4.88083	HN	113	GLN	HN	6 740
HB	110	ILE	HG1	4.96950	HA	112	ALA	QB	3.498470
HB	110	ILE	QD1	4.614400	HA	113	GLN	HN	3.2100400
HB	111	VAL	HN	3.565530	HA	127	VAL	HA	3.168920
HB	128	LEU	HN	6 3186	HA	127	VAL	QG1	7 1110
HB	129	ALA	HA	6 1170	HA	127	VAL	QG2	7 5014
HB	129	ALA	QB	7 4061	HA	128	LEU	HN	3.533630
QG2	110	ILE	HG1	3.661290	QB	113	GLN	HN	4 14060
QG2	110	ILE	HG1	4.224770	QB	124	ALA	QB	6.616180
QG2	110	ILE	QD1	5 36330	QB	126	GLU	HN	7 2250
QG2	111	VAL	HN	5.516910	QB	127	VAL	HA	6.76426
QG2	129	ALA	HA	5.713960	QB	127	VAL	HB	4.736770
QG2	129	ALA	QB	6.221570	QB	127	VAL	QG1	5.833740
QG2	130	LYS	HN	7 2820	QB	127	VAL	QG2	6.418220
HG12	110	ILE	QD1	4.5	QB	128	LEU	QD2	6.223120
16700					113	GLN			
HG12	111	VAL	HN	5	HN	113	GLN	HA	3.931820
41110					HN	113	GLN	HB2	4.122630
HG13	110	ILE	QD1	3.8	HN	113	GLN	HB3	3.933220
50290					HN	113	GLN	HG2	6 1168
HG13	111	VAL	HN	5.8	HN	113	GLN	HG3	6 707
16320					HN	124	ALA	QB	7 3937
QD1	111	VAL	HN	5.123730	HN	125	THR	HN	6 979
QD1	112	ALA	HN	7 3020	HN	126	GLU	HN	3.436100
QD1	112	ALA	QB	6.223120	HN	126	GLU	HB2	6 4953
QD1	127	VAL	QG2	7.110380	HN	126	GLU	HB3	6 2972
QD1	129	ALA	HA	7 4340	HN	127	VAL	HA	3.626080
QD1	129	ALA	QB	6.517020	HA	113	GLN	HB2	4.221680
111 VAL					HA	113	GLN	HB3	4.125340
HN	111	VAL	HA	4.123520	HA	113	GLN	HG2	4.315810
HN	111	VAL	HB	4.514040	HA	113	GLN	HG3	4.412560
HN	111	VAL	QG1	5 8298	HA	114	GLY	HN	3.2104900
HN	111	VAL	QG2	5 9314	HB2	113	GLN	HG2	4.217000
HN	112	ALA	HN	5.44694	HB2	113	GLN	HG3	4.412290
HN	128	LEU	HN	3.439460	HB2	113	GLN	HE2	4.69516
HN	128	LEU	HB2	5.522490	HB2	113	GLN	HE2	4.511050
HN	129	ALA	HA	3.819400	HB2	114	GLY	HN	4.514240
HN	129	ALA	QB	7 3297	HB2	126	GLU	HN	6 5134
HN	130	LYS	HN	5.61991	HB3	113	GLN	HG2	3.926860
HA	111	VAL	HB	4.414940	HB3	113	GLN	HG3	3.461900
HA	111	VAL	QG1	3.850080	HB3	113	GLN	HE2	4.69517
HA	111	VAL	QG2	4.227130	HB3	113	GLN	HE2	4.610380
HA	112	ALA	HN	3.1133300	HB3	114	GLY	HN	5 7541
HB	111	VAL	QG1	3.843600	HB3	125	THR	HN	6 877
HB	111	VAL	QG2	3.758050	HB3	126	GLU	HN	6 2374
HB	112	ALA	HN	4.318620	HG2	113	GLN	HE2	3.925710
HB	128	LEU	HN	6 960	HG2	113	GLN	HE2	5.15343
QG1	112	ALA	HN	6.110080	HG2	114	GLY	HN	5.913940
QG1	130	LYS	QE	8	HG3	113	GLN	HE2	4.78510
2263.0*2					HG3	113	GLN	HE2	5.43947
QG2	112	ALA	HN	5 26470	HG3	114	GLY	HN	5.816610
QG2	128	LEU	HN	7 1783	HE21	126	GLU	HB2	6 6194
QG2	128	LEU	HB3	5.616060	HE21	126	GLU	HG2	6 3635
QG2	128	LEU	QD2	7.95423	HE21	126	GLU	HG3	6 6032
					HE22	126	GLU	HN	6 4272

114	HE22	126	GLU	HB2	6	4114	HB2	116	LEU	QD2	3.941110	
	HE22	126	GLU	HB3	6	3755	HB2	117	GLY	HN	5.25458	
	HE22	126	GLU	HG2	6	1393	HB2	122	LEU	QD2	6.86009	
	HE22	126	GLU	HG3	6	1829	HB2	123	ALA	HN	5.815730	
	GLY						HB3	116	LEU	HG	3.467060	
	HN	114	GLY	HA1	3.840030		HB3	116	LEU	QD1	4.420070	
	HN	114	GLY	HA2	3.931610		HB3	116	LEU	QD2	4.517350	
	HN	115	VAL	HN	4.416690		HB3	117	GLY	HN	4.220150	
	HN	122	LEU	QD1	6.95616		HG	116	LEU	QD1	3.758560	
	HA1	115	VAL	HN	3.841440		HG	116	LEU	QD2	3.496460	
	HA1	116	LEU	QD2	7	4175	HG	117	GLY	HN	5.717800	
	HA1	124	ALA	HA	4.66581		QD1	117	GLY	HN	5.320600	
	HA1	124	ALA	QB	7	1973	QD1	118	GLU	HN	7	1697
	HA1	125	THR	HN	3.820750		QD1	120	GLY	HN	6.95554	
	HA2	115	VAL	HN	3.475440		QD1	121	LYS	HN	7	1217
	HA2	116	LEU	QD2	7	4691	QD1	122	LEU	HA	7	4215
	HA2	124	ALA	HA	4.47745		QD1	122	LEU	HB2	7	3658
	HA2	124	ALA	QB	7	1957	QD1	122	LEU	HG	5.615770	
	HA2	125	THR	HN	4.75571		QD1	123	ALA	HN	7	2932
	115	VAL						QD2	117	GLY	HN	6.38487
HN		115	VAL	HA	3.837210		QD2	122	LEU	HA	6	10950
HN		115	VAL	HB	3.743580		QD2	122	LEU	HB2	7	2192
HN		115	VAL	QG1	4	34580	QD2	122	LEU	HG	5.516410	
HN		115	VAL	QG2	5.36109		QD2	122	LEU	QD2	7	10960
HN		116	LEU	HN	4.710490		QD2	123	ALA	HN	6.47771	
HN		116	LEU	QD2	7	4794	117	GLY				
HN		122	LEU	QD1	7	1582		HN	117	GLY	HA1	3.746380
HN		123	ALA	HN	3.531870		HN	117	GLY	HA2	3.567760	
HN		124	ALA	HA	3.627870		HN	118	GLU	HN	4.220620	
	HN	124	ALA	QB	5.319900		HN	119	ASP	HN	6	1016
	HN	125	THR	QG2	7	1532	HN	120	GLY	HN	6	777
	HA	115	VAL	HB	4.415040		HN	121	LYS	HN	4.722960	
	HA	115	VAL	QG1	4.811980		HN	122	LEU	HA	3.436580	
	HA	115	VAL	QG2	4.614860		HN	122	LEU	HB3	6	4597
	HA	116	LEU	HN	3.1125400		HN	122	LEU	QD2	6	11310
	HB	115	VAL	QG1	4	35400	HN	123	ALA	HN	5.23120	
	HB	115	VAL	QG2	4.129550		HA1	118	GLU	HN	4.612760	
	HB	116	LEU	HN	4.710940		HA1	123	ALA	QB	7	4865
	QG1	116	LEU	HN	6.110370		HA2	118	GLU	HN	4.318490	
	QG1	123	ALA	QB	7.29112		HA2	119	ASP	HA	5.310440	
	QG2	116	LEU	HN	4.735910		HA2	123	ALA	QB	5.813120	
	QG2	123	ALA	HN	6.85690		118	GLU				
	LEU					HN		118	GLU	HA	4.416430	
	HN	116	LEU	HA	3.656360		HN	118	GLU	HB2	6	1239
	HN	116	LEU	HB2	3.561970		HN	118	GLU	HB3	5.44590	
	HN	116	LEU	HB3	4.221350		HN	118	GLU	QG	6.8	
	HN	116	LEU	HG	4.96910		2571.0*2					
	HN	116	LEU	QD1	5.64268			HN	119	ASP	HN	5.34845
	HN	116	LEU	QD2	4.99798		HN	122	LEU	QD1	7	1988
	HN	117	GLY	HN	4.98628		HA	118	GLU	HB2	3.2101900	
	HA	116	LEU	HB2	4.416980		HA	118	GLU	HB3	3.748980	
	HA	116	LEU	HB3	4.318020		HA	118	GLU	QG	4.8	
	HA	116	LEU	HG	4.315710		17930.0*2					
	HA	116	LEU	QD1	4.614930			HA	119	ASP	HN	3.742470
	HA	116	LEU	QD2	4.320620		HB2	118	GLU	QG	4.7	
	HA	117	GLY	HN	3.2117400		38265.0*2					
	HA	122	LEU	HA	3.256330			HB2	119	ASP	HN	4.612110
	HA	122	LEU	QD1	6.38668		HB2	121	LYS	HB2	4.852710	
	HA	122	LEU	QD2	6.76363		HB2	121	LYS	HB3	5.232970	
	HA	123	ALA	HN	3.256060		HB3	118	GLU	QG	4.3	
	HB2	116	LEU	HG	4.510800		69250.0*2					
	HB2	116	LEU	QD1	4	32610		HB3	119	ASP	HN	4.513640

	HB3	121	LYS	HB2	5	40440		QG	121	LYS	HD3	5.5
	HB3	121	LYS	HB3	5.3	27650	11440.0*2					
	QG	119	ASP	HN	7			QG	121	LYS	HE2	5.2
6170.0*2							18250.0*2					
119	ASP							QG	121	LYS	HE3	4.8
	HN	119	ASP	HA	3.9	34840	33885.0*2					
	HN	119	ASP	HB2	4.6	12570		QG	122	LEU	HN	7
	HN	120	GLY	HN	3.4	79040	11935.0*2					
	HN	120	GLY	HA1	5.9	2728		QG	122	LEU	QD1	5.8
	HN	120	GLY	HA2	6	1997	32835.0*2					
	HN	121	LYS	HN	5.1	12650	HD2	121	LYS	HE2	4.2	16520
	HA	119	ASP	HB2	3.4	71050	HD2	121	LYS	HE3	4.1	20330
	HA	120	GLY	HN	5.1	6724	HD2	122	LEU	HN	6	4065
	HB2	120	GLY	HN	5.6	3843	HD3	121	LYS	HE2	5.5	3341
120	GLY						HD3	121	LYS	HE3	5	5737
	HN	120	GLY	HA1	3.8	35910	HD3	122	LEU	HN	5.9	14820
	HN	120	GLY	HA2	3.4	75870	122	LEU				
	HN	121	LYS	HN	3.3	88290	HN	122	LEU	HA	4.1	25950
	HN	121	LYS	QG	7		HN	122	LEU	HB2	4.2	21690
1905.5*2							HN	122	LEU	HB3	4.3	17190
	HN	122	LEU	QD2	7	614	HN	122	LEU	HG	5.1	5578
	HA1	121	LYS	HN	4.4	16240	HN	122	LEU	QD1	5.7	3800
	HA1	122	LEU	QD1	7	2058	HN	122	LEU	QD2	5.6	4243
	HA2	121	LYS	HN	4.1	23220	HN	123	ALA	HN	5.3	5216
	HA2	122	LEU	QD1	7	2911	HA	122	LEU	HB2	5.1	6212
121	LYS						HA	122	LEU	HB3	4.8	9639
	HN	121	LYS	HA	4.2	21120	HA	122	LEU	HG	3.8	30870
	HN	121	LYS	HB2	3.8	40860	HA	122	LEU	QD1	4.4	19270
	HN	121	LYS	HB3	4	28080	HA	122	LEU	QD2	4.3	21430
	HN	121	LYS	QG	4.7		HA	123	ALA	HN	3.1	141600
40155.0*2							HA	123	ALA	QB	5.1	3353
	HN	121	LYS	HD2	5.4	3976	HB2	122	LEU	HG	3.7	37340
	HN	121	LYS	HD3	5.3	4127	HB2	122	LEU	QD1	4.4	18050
	HN	121	LYS	HE2	5.4	3947	HB2	122	LEU	QD2	4	34710
	HN	121	LYS	HE3	5.1	5074	HB3	122	LEU	HG	4.5	11800
	HN	122	LEU	HN	5.8	3006	HB3	122	LEU	QD1	5.1	7611
	HN	122	LEU	QD1	7	2748	HB3	122	LEU	QD2	3.8	47000
	HA	121	LYS	HB2	4.8	8801	HB3	123	ALA	HN	5.3	5190
	HA	121	LYS	HB3	3.9	35230	HG	122	LEU	QD1	3.5	70280
	HA	121	LYS	QG	5.6		HG	122	LEU	QD2	3.9	40980
6205.0*2							HG	123	ALA	HN	5.6	18940
	HA	121	LYS	HD2	4.6	10170	QD1	123	ALA	HN	7	3177
	HA	121	LYS	HD3	4.3	14810	QD1	123	ALA	QB	7.5	7044
	HA	121	LYS	HE3	5.3	4266	QD1	124	ALA	HN	7	2229
	HA	122	LEU	HN	3.3	84420	QD2	123	ALA	HN	6.1	10140
	HB2	121	LYS	QG	4.8		QD2	124	ALA	QB	7.9	5527
31980.0*2							123	ALA				
	HB2	121	LYS	HD2	4.1	21230	HN	123	ALA	HA	3.9	35660
	HB2	121	LYS	HD3	3.7	34790	HN	123	ALA	QB	3.4	89870
	HB2	121	LYS	HE2	6	2058	HN	124	ALA	HN	5	7224
	HB2	121	LYS	HE3	6	1996	HA	123	ALA	QB	3.4	51020
	HB2	122	LEU	HN	4.7	10970	HA	124	ALA	HN	3.2	102900
	HB3	121	LYS	QG	5.4		QB	124	ALA	HN	5	3641
12300.0*2							124	ALA				
	HB3	121	LYS	HD2	4.4	13410	HN	124	ALA	HA	4.1	26010
	HB3	121	LYS	HD3	4.1	21140	HN	124	ALA	QB	3.4	82770
	HB3	121	LYS	HE2	5.7	2755	HN	125	THR	HN	5.5	4318
	HB3	121	LYS	HE3	6	611	HA	124	ALA	QB	3.4	107000
	HB3	122	LEU	HN	3.7	42950	HA	125	THR	HN	3.4	71360
	QG	121	LYS	HD2	4.8		HA	126	GLU	HN	4.7	22840
31435.0*2							QB	125	THR	HN	4.5	7178
							QB	125	THR	HA	5.7	1726

125	QB	126	GLU	HN	4.74470		HA	128	LEU	HG	4	25060
	THR						HA	128	LEU	QD1	4.6	15380
	HN	125	THR	HA	3.836880		HA	128	LEU	QD2	5	9266
	HN	125	THR	HB	4.124120		HA	129	ALA	HN	4.2	21820
	HN	125	THR	QG2	5	8668	HA	129	ALA	QB	6.9	515
	HN	126	GLU	HN	3.392230		HB2	128	LEU	HG	4.4	13520
	HA	125	THR	HB	3.383300		HB2	128	LEU	QD1	4.5	15930
	HA	125	THR	QG2	3.939540		HB2	128	LEU	QD2	4.1	30650
	HA	125	THR	HG1	6	1445	HB2	129	ALA	HN	4.3	17720
	HA	126	GLU	HN	4.124090		HB3	128	LEU	HG	4.2	16340
126	HB	125	THR	QG2	4.322040		HB3	128	LEU	QD1	6.2	2350
	HB	126	GLU	HN	5	7368	HB3	128	LEU	QD2	4.3	22010
	QG2	126	GLU	HN	6.29135		HB3	129	ALA	HN	3.9	32730
	HG1	126	GLU	HA	6	1747	HG	128	LEU	QD1	4.3	23010
	HG1	127	VAL	QG2	7	1982	HG	128	LEU	QD2	3.9	42390
	GLU						HG	129	ALA	HN	6	11820
	HN	126	GLU	HA	4.122800		QD1	129	ALA	HN	5.7	14220
	HN	126	GLU	HB2	5.16344		QD2	129	ALA	HN	7	3527
	HN	126	GLU	HB3	3.836170		QD2	130	LYS	HN	7	3707
	HN	126	GLU	HG2	5.43815		QD2	130	LYS	QD	6.5	
127	HN	126	GLU	HG3	4.412630		17020.0*2					
	HN	127	VAL	HN	4.512980		129	ALA				
	HN	127	VAL	QG2	7	2411	HN	129	ALA	HA	4.1	25260
	HA	126	GLU	HB2	4.126200		HN	129	ALA	QB	3.8	19110
	HA	126	GLU	HB3	3.933580		HN	130	LYS	HN	4.7	11200
	HA	126	GLU	HG2	4.79283		HA	129	ALA	QB	3.4	93910
	HA	126	GLU	HG3	5.24856		HA	130	LYS	HN	3.3	90750
	HA	127	VAL	HN	3.482820		HA	130	LYS	QG	6.2	
	HA	127	VAL	QG2	7	1042	30130.0*2					
	HB2	126	GLU	HG2	4	23130	QB	130	LYS	HN	4.5	6877
128	HB2	126	GLU	HG3	3.738450		QB	130	LYS	HB2	7	2399
	HB2	127	VAL	HN	4.611520		QB	131	HIS	HN	4.9	3161
	HB3	126	GLU	HG2	4.120340		130	LYS				
	HB3	126	GLU	HG3	4.217150		HN	130	LYS	HA	4.2	22180
	HB3	127	VAL	HN	4.513770		HN	130	LYS	HB2	4	28640
	HG2	127	VAL	HN	5.915030		HN	130	LYS	HB3	4.1	23700
	HG3	127	VAL	HN	6	2417	HN	130	LYS	QG	6.3	
	VAL						4241.5*2					
	HN	127	VAL	HA	4.124200		HN	130	LYS	QD	5.1	
	HN	127	VAL	HB	4	29080	19995.0*2					
	HN	127	VAL	QG1	5	8996	HN	130	LYS	QE	7	0.0*2
129	HN	127	VAL	QG2	4.224280		HA	130	LYS	HB2	4.3	17430
	HN	128	LEU	HN	5.73447		HA	130	LYS	HB3	4.7	10260
	HA	127	VAL	HB	4.711050		HA	130	LYS	QG	5.3	
	HA	127	VAL	QG1	3.939880		9030.0*2					
	HA	127	VAL	QG2	4	32370	HA	130	LYS	QD	5.6	
	HA	128	LEU	HN	3.1139500		10130.0*2					
	HB	127	VAL	QG1	3.845700		HA	130	LYS	QE	7	
	HB	127	VAL	QG2	3.4183600		1893.0*2					
	HB	128	LEU	HN	4.98064		HA	131	HIS	HN	3.7	46160
	QG1	128	LEU	HN	5.124950		HB2	130	LYS	QG	4.8	
130	QG2	128	LEU	HN	6.48118		32080.0*2					
	LEU						HB2	130	LYS	QD	6.3	
	HN	128	LEU	HA	4.318440		4326.0*2					
	HN	128	LEU	HB2	4	30170	HB2	130	LYS	QE	7	
	HN	128	LEU	HB3	4.612340		428.0*2					
	HN	128	LEU	HG	4.69861		HB3	130	LYS	QG	4.4	
	HN	128	LEU	QD1	4.811570		62900.0*2					
	HN	128	LEU	QD2	5	8947	HB3	130	LYS	QD	6.1	
	HN	129	ALA	HN	4.611550		5190.0*2					
	HA	128	LEU	HB2	5.16748		HB3	130	LYS	QE	7	
131	HA	128	LEU	HB3	3.654940		1672.5*2					

QG	130	LYS	QD	6.5		HN	135	TYR	CZ	7	
11442.5*4						632.5*2					
QG	130	LYS	QE	6.9		HA	135	TYR	HB2	4	27250
7097.5*4						HA	135	TYR	HB3	4.3	19230
QD	130	LYS	QE	6.5		HA	135	TYR	CG	6.4	
10765.0*4						3985.5*2					
QE	131	HIS	HD2	7		HA	135	TYR	CZ	6.6	0.0*2
8280.0*2						HB2	135	TYR	CG	6.5	
131	HIS					11505.0*2					
HN	131	HIS	HA	6	2022	HB2	135	TYR	CZ	8	
HN	132	ASP	HN	4.2	21430	1762.5*2					
HA	132	ASP	HN	4.1	24610	HB3	135	TYR	CG	6.6	
HB2	132	ASP	HN	6	1452	9930.0*2					
HB3	131	HIS	HD2	5.1	5449	HB3	135	TYR	CZ	7.9	
HB3	132	ASP	HN	4.7	10100	2279.5*2					
132	ASP					CG	135	TYR	CZ	7.6	
HN	132	ASP	HA	4	26860	46800.0*4					
HN	133	GLU	HN	4.3	18620						
HA	133	GLU	HN	3.9	32620						
133	GLU										
HN	133	GLU	HA	4.4	15680						
HN	133	GLU	HB2	3.8	36490						
HN	133	GLU	HB3	3.8	38850						
HN	133	GLU	QG	5.1							
20335.0*2											
HN	134	ASN	HN	4.4	15430						
HN	134	ASN	HA	4.7	10170						
HN	134	ASN	HB3	5	7034						
HA	133	GLU	HB2	4	29380						
HA	133	GLU	HB3	3.8	36740						
HA	133	GLU	QG	5.4							
8155.0*2											
HA	134	ASN	HN	3.6	57890						
HB2	133	GLU	QG	4.8							
33290.0*2											
HB2	134	ASN	HN	5.1	6654						
HB3	133	GLU	QG	4.6							
46165.0*2											
HB3	134	ASN	HN	6	762						
134	ASN										
HN	134	ASN	HA	3.6	51440						
HN	134	ASN	HB2	4.4	16680						
HN	134	ASN	HB3	4	28780						
HN	134	ASN	HD2	4.9	6657						
HN	134	ASN	HD2	4.8	7987						
HN	135	TYR	HN	4.6	11980						
HA	134	ASN	HB2	4	27300						
HA	134	ASN	HB3	4.4	16080						
HA	134	ASN	HD2	6	1002						
HA	134	ASN	HD2	6	991						
HA	135	TYR	HN	3.8	38360						
HB2	134	ASN	HD2	5	6100						
HB2	134	ASN	HD2	5.2	4583						
HB3	134	ASN	HD2	4	25220						
HB3	134	ASN	HD2	5	5923						
HD22	135	TYR	HB2	6	6378						
135											