SUPPORTING INFORMATION

Structure and dynamics of reduced *Bacillus pasteurii* cytochrome *c*: oxidation state dependent properties and implications for electron transfer processes[†]

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Table 1: ¹⁵N and ¹H NMR chemical shifts in the reduced cytochrome *c* from *Bacillus pasteurii* (T=296 K).

Table 2: Upper distance limits used in solution structure calculations.

Table 3: Dihedral angle constraints used in solution structure calculations.

Table 4: N¹⁵ relaxation data of reduced cytochrome *c* from *Bacillus pasteurii* (T=296 K at 500 MHz).

Table 5: . The ratio of the opening constants (K^{op}) determined in the two oxidation states is shown on a per residue basis

Figure 1: ¹⁵N and ¹H HSQC spectrum of reduced recombinant cytochrome *c* from *Bacillus pasteurii* at pH 7.

Table 1: ^{15}N and ^1H NMR chemical shifts of amino acid residues in the reduced cytochrome *c* from *Bacillus pasteurii* (T=296 K). The stereospecific assignments are underlined.

Residue	Nr.	N	H^{N}	H^{α}	H^{β}	Others
VAL	22			3.87	1.74	$\gamma\text{-CH}_3$ (0.71,0.79)
ASP	23	126.55	8.49	4.48	2.38, 2.77	
ALA	24	126.91	8.28	3.42	0.89	
GLU	25	115.03	7.59	2.60	1.55, 1.71	γ (1.89, 1.96)
ALA	26	120.43	7.06	3.91	1.28	
VAL	27	118.87	7.55	3.57	1.96	$\gamma\text{-CH}_3$ (0.79, 0.86)
VAL	28	120.55	8.09	4.01	1.88	$\gamma\text{-CH}_3$ (0.76, 1.02)
GLN	29		7.83	3.86	<u>2.02, 2.07</u>	γ (2.34, 2.38) $\epsilon\text{-N}$ (111.91) ϵ (6.83, 7.42)
GLN	30		7.64	4.21	2.16, 2.18	γ (2.33, 2.49) $\epsilon\text{-N}$ (110.95) ϵ (6.77, 7.40)
LYS	31		8.76	4.86	2.17, 2.26	γ (1.51, 1.55) δ (1.64, 1.80) $\epsilon\text{-CH}_3$ (3.06)
CYS	32	114.98	8.77	6.04	<u>2.45, 2.58</u>	
ILE	33		6.96	3.20	1.29	$\gamma\text{-CH}_2$ (1.04) $\gamma\text{-CH}_3$ (0.79) $\delta\text{-CH}_3$ (0.15)
SER	34	119.35	8.52	3.87	3.83, 3.90	
CYS	35	114.67	6.10	4.37	<u>2.06, 0.74</u>	
HIS	36		6.12	2.58	<u>1.30, 0.87</u>	δ (0.47) ϵ (0.50) $\delta\text{-HN}$ (9.56) $\delta\text{-N}$ (164.58)
GLY	37	106.75	7.08	<u>3.20, 3.92</u>		
GLY	38	108.07	8.31	3.44, 3.67		
ASP	39	115.87	7.42	4.46	<u>2.36, 2.78</u>	
LEU	40		7.46	3.15	<u>1.01, 1.07</u>	γ (1.79) $\delta\text{-CH}_3$ (0.15, 0.62)
THR	41	105.67	7.39	3.95	4.25	$\gamma\text{-CH}_3$ (0.81)
GLY	42	111.31	7.61	<u>2.60, 3.98</u>		
ALA	43	125.59	7.48	3.98	0.82	
SER	44	118.63	7.76	4.08	<u>3.78, 3.91</u>	
ALA	45	125.11	7.30	4.17	-1.64	
PRO	46	--		3.91	2.12, 2.17	γ (1.48, 1.786) δ (2.41, 3.49)
ALA	47	120.31	7.92	3.37	1.10	
ILE	48		7.77	4.17	1.82	γ (- 0.95,-1.37) $\gamma\text{-CH}_3$ (- 0.84) $\delta\text{-CH}_3$ (0.41)
ASP	49	119.98	8.25	3.60	<u>2.13, 2.31</u>	
LYS	50		7.72	4.22	1.17, 1.69	γ (0.86, 0.98) δ (1.26, 1.42) $\epsilon\text{-CH}_3$ (2.72)
ALA	51	121.03	7.13	4.24	1.55	
GLY	52	103.99	8.29	<u>3.67, 4.37</u>		
ALA	53	120.67	7.97	4.16	1.40	
ASN	54	113.35	7.49	4.59	<u>2.21, 2.34</u>	δ (6.74, 7.25)

						δ -N(113.59)
TYR	55	118.27	8.07	5.02	<u>2.58, 3.32</u>	δ -CH ₂ (7.29) ϵ -CH ₂ (6.97)
SER	56	114.91	9.11	4.56	3.96, 4.35	
GLU	57	121.63	9.02	3.67	1.85, 1.99	γ -CH ₂ (1.89)
GLU	58	116.23	8.68	3.81	1.83, 1.91	γ (2.19, 2.25)
GLU	59	120.07	7.71	3.94	<u>2.04, 2.62</u>	γ (2.30, 2.35)
ILE	60	119.71	8.37	3.36	1.91	γ -CH ₃ (0.76) γ -CH ₂ (1.18) δ -CH ₃ (0.68)
LEU	61	119.71	8.38	3.69	<u>1.19, 1.84</u>	γ (1.40) δ -CH ₃ (0.64, 0.80)
ASP	62	116.59	7.41	4.01	<u>2.50, 2.54</u>	
ILE	63	120.43	7.24	2.54	1.26	γ -CH ₃ (-1.22) γ (0.25, 1.31) δ -CH ₃ (0.15)
ILE	64	116.23	7.55	2.25	1.47	γ -CH ₃ (0.48) γ (0.38, 1.74) δ -CH ₃ (0.93)
LEU	65	115.63	8.56	3.70	1.02, 1.49	γ (0.65) δ -CH ₃ (0.49, 1.58)
ASN	66	112.51	8.20	4.46	<u>2.39, 2.46</u>	δ (6.76, 7.5) δ -N(115.99)
GLY	67	111.91	7.48	2.06, 3.21		
GLN	68	114.55	6.47	3.73	<u>0.88, 1.61</u>	γ (1.82, 1.90) ϵ (6.88, 8.55) ϵ -N (110.80)
GLY	69	115.15	8.68	3.44, 3.74		
GLY	70	114.79	9.62	<u>3.85, 3.98</u>		
MET	71	125.23	8.10	3.06	<u>-0.59, -2.70</u>	γ (-1.77, 3.55) ϵ -CH ₃ (-3.18)
PRO	72	--		3.74	1.85	γ -CH ₂ (1.26) δ -CH ₂ (7.67)
GLY	73	103.4	7.67	2.66, 3.06		
GLY	74	106.03	7.53	<u>3.37, 3.56</u>		
ILE	75	124.15	9.50	3.37	1.63	γ (0.79, 0.88) γ -CH ₃ (1.30) δ -CH ₃ (0.40)
ALA	76	113.95	6.62	4.42	0.89	
LYS	77	114.79	8.42	4.32	1.43, 1.65	γ -CH ₂ (1.40) δ -CH ₂ (1.13) ϵ -CH ₂ (2.81)
GLY	78	107.59	8.42	3.64, 3.74		
ALA	79	127.15	8.69	4.04	1.35	
GLU	80	117.91	8.20	3.89	2.04, 2.28	γ (2.40, 2.46)
ALA	81	120.19	6.82	3.52	0.95	
GLU	82	114.91	7.94	3.73	<u>1.91, 1.95</u>	γ (2.11, 2.28)
ALA	83	120.67	7.91	4.19	1.44	
VAL	84	119.23	8.13	3.61	2.13	γ -CH ₃ (1.10, 1.21)
ALA	85	121.75	8.60	4.08	1.49	
ALA	86	117.31	7.69	3.86	1.44	
TRP	87	119.23	7.81	4.18	<u>3.15, 3.38</u>	δ (7.33) ζ (6.73, 7.33) η (7.02) ϵ -HN (10.21) ϵ (7.34) ϵ -N (130.14)
LEU	88	118.63	9.07	3.76	<u>1.70, 2.01</u>	γ (2.13) δ -CH ₃ (1.10, 1.22)
ALA	89	118.03	8.10	3.78	1.49	

GLU	90	111.67	6.71	4.09	1.74, 2.09	γ (2.16, 2.37)
LYS	91	122.83	7.46	3.98	1.70, 1.89	γ (0.83, 1.40) δ -CH ₂ (1.58) ϵ -CH ₂ (2.12)
LYS	92	126.19	7.19	3.98	1.39, 1.59	γ -CH ₂ (0.97) δ -CH ₂ (0.90) ϵ -CH ₂ (2.82)

Heme Assignments

QM1 (3.30) QM8 (2.94) HDM (8.99) HT2A (5.83) QT2 (1.82) HAM (9.79) QM3 (3.77) QT4 (2.19) HT4A (6.25)
HBM (9.37) QM5 (3.30) HGM (9.58) HAP61 (4.31) HAP62 (3.85) HBP63 (3.07) HBP64 (2.82) HAP71 (4.39)
HAP72 (4.49) HBP73 (3.17) HBP74 (2.94)

Table 2: Upper distance limits used in solution structure calculations

VAL 22					
HA	22	VAL	HB	4.5	
HA	22	VAL	QG1	4.3	
HA	22	VAL	QG2	4.9	
HA	23	ASP-	HN	3.4	
HB	22	VAL	QG1	5.1	
HB	22	VAL	QG2	4.3	
HB	23	ASP-	HN	5.9	
HB	27	VAL	QG2	5.2	
HB	79	ALA	QB	6.2	
HB	83	ALA	QB	5.3	
QG1	27	VAL	HN	7	
QG1	80	GLU-	HB2	6	
QG2	23	ASP-	HN	6.2	
QG2	80	GLU-	HA	6	
QG2	80	GLU-	HG3	6.8	
QG2	83	ALA	QB	6.2	
23 ASP-					
HN	23	ASP-	HA	4.5	
HN	23	ASP-	HB2	3.9	
HN	23	ASP-	HB3	4.2	
HN	24	ALA	HN	5.2	
HN	24	ALA	HA	5.3	
HN	26	ALA	HN	6	
HN	26	ALA	QB	5.8	
HN	27	VAL	QG2	7	
HA	23	ASP-	HB2	4.3	
HA	23	ASP-	HB3	3.8	
HA	24	ALA	HN	3.4	
HA	24	ALA	HA	6	
HA	24	ALA	QB	5.5	
HA	25	GLU-	HN	5.2	
HA	26	ALA	HN	6	
HA	26	ALA	QB	7	
HB2	24	ALA	HN	5.9	
HB2	26	ALA	HN	4.8	
HB2	26	ALA	QB	5.3	
HB2	27	VAL	HN	6	
HB3	24	ALA	HN	5.5	
HB3	25	GLU-	HN	5.2	
HB3	26	ALA	HN	5.6	
HB3	26	ALA	QB	6.4	
HB3	27	VAL	HN	4.9	
24 ALA					
HN	24	ALA	HA	4.1	
HN	24	ALA	QB	3.4	
HN	25	GLU-	HN	4.2	

	HN	26	ALA	HN	5.8
	HN	83	ALA	QB	7
	HN	87	TRP	HD1	6
	HA	24	ALA	QB	3.6
	HA	25	GLU-	HN	5
	HA	26	ALA	HN	5.6
	HA	27	VAL	HN	4.5
	HA	27	VAL	HB	3.9
	HA	27	VAL	QG1	5.6
	HA	27	VAL	QG2	6.4
	HA	28	VAL	HN	5.6
	HA	28	VAL	QG2	6.3
	HA	83	ALA	QB	7
	HA	84	VAL	HN	6
	HA	84	VAL	QG2	5.7
	HA	87	TRP	HD1	6
	QB	25	GLU-	HN	4
	QB	26	ALA	HN	5.4
	QB	28	VAL	QG2	5.2
	QB	83	ALA	HA	6.9
	QB	83	ALA	QB	6.4
	QB	84	VAL	HN	7
	QB	84	VAL	HA	5.1
	QB	87	TRP	HN	7
	QB	87	TRP	HB2	5.6
	QB	87	TRP	HB3	5.4
	QB	87	TRP	HD1	6
	QB	87	TRP	HE3	6.4
	QB	87	TRP	HE1	7
25	GLU-				
	HN	25	GLU-	HA	4
	HN	25	GLU-	HB2	3.4
	HN	25	GLU-	HB3	3.7
	HN	25	GLU-	HG2	5.9
	HN	25	GLU-	HG3	6
	HN	26	ALA	HN	3.9
	HN	87	TRP	HD1	5.8
	HN	87	TRP	HE1	6
	HA	25	GLU-	HB2	4.1
	HA	25	GLU-	HB3	3.8
	HA	25	GLU-	HG2	4.9
	HA	25	GLU-	HG3	4.6
	HA	26	ALA	HN	4.6
	HA	26	ALA	HA	6
	HA	28	VAL	HN	4.9
	HA	28	VAL	HB	4.1
	HA	28	VAL	QG1	6.7
	HA	28	VAL	QG2	6.2
	HA	29	GLN	HN	5.5
	HA	87	TRP	HE1	6
	HA	87	TRP	HZ2	5.4
	HA	87	TRP	HH2	5.6

	HB2	25	GLU-	HG2	5
	HB2	26	ALA	HN	4.1
	HB2	87	TRP	HE1	6
	HB2	87	TRP	HZ2	5.4
	HB2	87	TRP	HH2	5.9
	HB3	25	GLU-	HG2	5.5
	HB3	26	ALA	HN	4.5
	HB3	28	VAL	HB	4.3
	HB3	87	TRP	HE1	5.1
	HB3	87	TRP	HZ2	4.7
	HB3	87	TRP	HH2	6
	HG2	26	ALA	HN	5.5
	HG2	29	GLN	HB3	4.1
	HG2	87	TRP	HD1	4.9
	HG2	87	TRP	HE1	6
	HG2	87	TRP	HH2	5.5
	HG3	26	ALA	HN	6
	HG3	29	GLN	HB2	3.1
	HG3	87	TRP	HE1	6
	HG3	87	TRP	HZ2	5.6
26 ALA	HN	26	ALA	HA	3.9
	HN	26	ALA	QB	3.4
	HN	27	VAL	HN	3.4
	HN	27	VAL	HA	6
	HN	28	VAL	HN	5.6
	HN	29	GLN	HN	5.7
	HA	26	ALA	QB	3.4
	HA	27	VAL	HN	5
	HA	28	VAL	HN	5.8
	HA	29	GLN	HN	4.5
	HA	29	GLN	HB2	3.8
	HA	29	GLN	HB3	3.9
	HA	29	GLN	HG2	5.5
	HA	29	GLN	HG3	5.2
	QB	27	VAL	HN	3.7
	QB	27	VAL	HA	5.8
	QB	27	VAL	QG2	7.6
	QB	29	GLN	HN	6.5
27 VAL	HN	27	VAL	HA	4.1
	HN	27	VAL	HB	3.6
	HN	27	VAL	QG1	4.3
	HN	27	VAL	QG2	5.6
	HN	28	VAL	HN	3.9
	HN	29	GLN	HN	4.4
	HN	84	VAL	QG2	7
	HA	27	VAL	HB	4.5
	HA	27	VAL	QG1	4.5
	HA	27	VAL	QG2	4.5
	HA	28	VAL	HN	5
	HA	29	GLN	HN	5.8

	HA	30	GLN	HN	4.5
	HA	30	GLN	HB2	4
	HA	30	GLN	HB3	4.1
	HA	31	LYS+	HN	6
	HA	31	LYS+	HB2	4.1
	HA	31	LYS+	HB3	4.7
	HA	31	LYS+	HD3	4.8
	HA	31	LYS+	QE	7
	HB	27	VAL	QG1	3.9
	HB	27	VAL	QG2	4.2
	HB	28	VAL	HN	3.7
	HB	28	VAL	QG2	6.8
	HB	84	VAL	QG2	4.9
	QG1	28	VAL	HN	6.9
	QG1	28	VAL	QG2	5.9
	QG1	31	LYS+	HD3	6.6
	QG1	75	ILE	QG2	6
	QG1	80	GLU-	HA	6.9
	QG1	80	GLU-	HB3	5.7
	QG1	93	HEM	QT2	6.2
	QG2	28	VAL	HN	6.6
	QG2	31	LYS+	QE	8
	QG2	76	ALA	QB	5.4
	QG2	80	GLU-	HA	5.7
	QG2	80	GLU-	HB3	5.4
	QG2	83	ALA	QB	7.1
28 VAL					
	HN	28	VAL	HA	4.2
	HN	28	VAL	HB	3.6
	HN	28	VAL	QG1	4.4
	HN	28	VAL	QG2	4.9
	HN	29	GLN	HN	4.2
	HN	30	GLN	HN	5.6
	HN	84	VAL	QG1	7
	HN	84	VAL	QG2	6
	HN	87	TRP	HZ2	6
	HA	28	VAL	HB	4.2
	HA	28	VAL	QG1	6.4
	HA	28	VAL	QG2	4.6
	HA	29	GLN	HN	5.5
	HA	30	GLN	HN	5.5
	HA	31	LYS+	HN	4.5
	HA	32	CYSS	HN	4.6
	HA	32	CYSS	HB2	4.1
	HA	33	ILE	HN	6
	HB	28	VAL	QG1	4
	HB	28	VAL	QG2	4
	HB	29	GLN	HN	3.9
	HB	29	GLN	HG2	5.1
	HB	87	TRP	HE3	6
	HB	87	TRP	HZ3	5.7
	HB	87	TRP	HH2	5.7

	QG1	29	GLN	HN	7
	QG1	29	GLN	HE21	7
	QG1	32	CYSS	HN	7
	QG1	32	CYSS	HB2	7
	QG1	32	CYSS	HB3	7
	QG1	40	LEU	HG	5
	QG1	40	LEU	QD2	6.1
	QG1	48	ILE	HG12	6.4
	QG1	84	VAL	QG1	5.6
	QG1	87	TRP	HE3	5.9
	QG1	87	TRP	HZ3	5.7
	QG1	87	TRP	HH2	6.7
	QG1	88	LEU	QD1	7.3
	QG1	88	LEU	QD2	5.2
	QG1	93	HEM	QM1	7
	QG2	29	GLN	HN	6.5
	QG2	32	CYSS	HN	7
	QG2	32	CYSS	HB2	5.7
	QG2	32	CYSS	HB3	6.1
	QG2	40	LEU	QD1	6.1
	QG2	40	LEU	QD2	5.5
	QG2	48	ILE	HG12	6.8
	QG2	87	TRP	HE3	7
	QG2	87	TRP	HZ3	5.8
	QG2	87	TRP	HH2	6.5
	QG2	93	HEM	QT2	7
29 GLN					
	HN	29	GLN	HA	4.4
	HN	29	GLN	HB2	3.7
	HN	29	GLN	HB3	4.2
	HN	29	GLN	HG2	5.4
	HN	29	GLN	HG3	5.6
	HN	29	GLN	HE21	6
	HN	30	GLN	HN	3.8
	HN	31	LYS+	HN	6
	HN	32	CYSS	HN	6
	HN	33	ILE	QG2	7
	HA	29	GLN	HB2	4
	HA	29	GLN	HB3	4.1
	HA	29	GLN	HG2	5.9
	HA	29	GLN	HG3	6
	HA	30	GLN	HN	5
	HA	31	LYS+	HN	6
	HA	33	ILE	HN	6
	HA	33	ILE	HB	4.9
	HA	33	ILE	QG2	5.5
	HA	33	ILE	QG1	6.6
	HB2	30	GLN	HN	4.9
	HB2	33	ILE	QG2	5.5
	HB3	30	GLN	HN	4.6
	HB3	33	ILE	QG2	5.4
	HG2	29	GLN	HE21	5.3

	HG2	29	GLN	HE22	6
	HG3	29	GLN	HE21	5.2
	HG3	29	GLN	HE22	6
	HE21	33	ILE	QG2	6.6
	HE21	33	ILE	QG1	7
	HE21	38	GLY	HA1	6
	HE21	40	LEU	QD1	7
	HE21	87	TRP	HH2	5.7
	HE22	33	ILE	QG2	6.4
	HE22	38	GLY	HA2	6
	HE22	87	TRP	HH2	5.1
30 GLN					
	HN	30	GLN	HA	4.2
	HN	30	GLN	HB2	3.7
	HN	30	GLN	HB3	3.9
	HN	30	GLN	HG2	5.6
	HN	30	GLN	HG3	5.7
	HN	31	LYS+	HN	4.1
	HN	31	LYS+	HA	6
	HN	32	CYSS	HN	4
	HN	33	ILE	HN	6
	HN	33	ILE	QG2	7
	HA	30	GLN	HB2	3.9
	HA	30	GLN	HB3	4
	HA	30	GLN	HG2	6
	HA	30	GLN	HG3	5.6
	HA	30	GLN	QG	6.6
	HA	31	LYS+	HN	5.9
	HA	32	CYSS	HN	6
	HA	33	ILE	QG2	7
	HB2	30	GLN	HG2	5.4
	HB2	30	GLN	HG3	3.8
	HB3	30	GLN	HG2	5.4
	HG3	30	GLN	QG	5.1
	HE22	31	LYS+	HG3	6
31 LYS+					
	HN	31	LYS+	HA	4.2
	HN	31	LYS+	HB2	3.8
	HN	31	LYS+	HB3	3.6
	HN	31	LYS+	HG2	6
	HN	31	LYS+	HG3	6
	HN	31	LYS+	HD3	5.4
	HN	31	LYS+	QE	7
	HN	33	ILE	HN	3.8
	HN	93	HEM	HT2A	6
	HN	93	HEM	QT2	7
	HA	31	LYS+	HB2	4.1
	HA	31	LYS+	HB3	3.6
	HA	31	LYS+	HG2	5.8
	HA	31	LYS+	HG3	4.8
	HA	31	LYS+	HD2	5.8
	HA	31	LYS+	HD3	5.3

HA	31	LYS+	QE	7
HA	32	CYSS	HN	4.8
HA	75	ILE	QG2	7
HB2	31	LYS+	HG3	4.9
HB2	31	LYS+	HD3	4.9
HB2	31	LYS+	QE	7
HB2	32	CYSS	HA	6
HB2	75	ILE	QG2	6
HB2	93	HEM	HT2A	5.9
HB3	31	LYS+	HG3	4.2
HB3	31	LYS+	HD3	4.3
HB3	31	LYS+	QE	7
HB3	32	CYSS	HN	4.2
HB3	32	CYSS	HA	6
HB3	75	ILE	QG2	5.3
HB3	93	HEM	HT2A	5.8
HG2	31	LYS+	QE	7
HG3	31	LYS+	QE	6.2
HD2	31	LYS+	QE	6.4
HD3	31	LYS+	QE	6.4
HD3	75	ILE	QG2	6
HD3	93	HEM	HT2A	6
QE	75	ILE	HA	7
QE	75	ILE	QG2	8
QE	75	ILE	HG12	7
QE	76	ALA	HA	7
QE	76	ALA	QB	8
32 CYSS				
HN	32	CYSS	HA	4.4
HN	32	CYSS	HB2	4.2
HN	32	CYSS	HB3	4.8
HN	33	ILE	HN	4.2
HN	33	ILE	HB	6
HN	33	ILE	QG2	6.8
HN	33	ILE	QG1	7
HN	34	SER	HN	5.6
HN	93	HEM	HT2A	6
HN	93	HEM	HAM	6
HA	32	CYSS	HB2	4.2
HA	32	CYSS	HB3	4
HA	33	ILE	HN	5.9
HA	34	SER	HN	6
HA	36	HIS	HD2	5.4
HA	75	ILE	QG2	7
HA	75	ILE	QD1	7
HA	93	HEM	HT2A	4.3
HA	93	HEM	QT2	7
HA	93	HEM	HAM	3.8
HA	93	HEM	QM3	6.1
HB2	33	ILE	HN	5.1
HB2	33	ILE	QG2	6.9
HB2	36	HIS	HD2	5.9

	HB2	48	ILE	HG12	6
	HB2	93	HEM	QM1	7
	HB2	93	HEM	HT2A	5.5
	HB2	93	HEM	HAM	6
	HB3	33	ILE	HN	5.8
	HB3	36	HIS	HB2	4.2
	HB3	36	HIS	HD2	4.7
	HB3	93	HEM	QM1	6
	HB3	93	HEM	HT2A	5.2
	HB3	93	HEM	HAM	5.6
33 ILE					
	HN	33	ILE	HA	4.2
	HN	33	ILE	HB	3.6
	HN	33	ILE	QG2	4.3
	HN	33	ILE	QG1	6.9
	HN	33	ILE	QD1	7
	HN	34	SER	HN	4.4
	HN	34	SER	HA	5.4
	HA	33	ILE	HB	3.8
	HA	33	ILE	QG2	4.4
	HA	33	ILE	QG1	6.6
	HA	33	ILE	QD1	5.8
	HA	34	SER	HN	5.7
	HA	35	CYSS	HN	5
	HA	36	HIS	HN	4.6
	HA	36	HIS	HB2	3.6
	HA	36	HIS	HB3	5
	HA	38	GLY	HA1	5.2
	HB	33	ILE	QG2	3.9
	HB	33	ILE	QG1	5.1
	HB	33	ILE	QD1	3.7
	HB	34	SER	HN	5.4
	HB	38	GLY	HN	6
	HB	38	GLY	HA2	4.7
	QG2	33	ILE	QD1	5.5
	QG2	38	GLY	HA1	7
	QG2	38	GLY	HA2	5.9
	QG2	40	LEU	HN	7
	QG2	40	LEU	QD1	7.5
	QG1	34	SER	HN	6.8
	QG1	38	GLY	HA2	7
34 SER					
	HN	34	SER	HA	3.9
	HN	34	SER	HB2	4.6
	HN	34	SER	HB3	4.4
	HN	35	CYSS	HN	5
	HN	36	HIS	HN	5.1
	HA	35	CYSS	HN	5.7
	HA	37	GLY	HN	5.9
	HB2	35	CYSS	HN	6
	HB2	36	HIS	HN	6
	HB2	93	HEM	QM3	5.7

	HB3	35	CYSS	HN	5.4
	HB3	93	HEM	QM3	5.5
35 CYSS					
	HN	35	CYSS	HA	4.9
	HN	35	CYSS	HB2	4.4
	HN	35	CYSS	HB3	4.1
	HN	36	HIS	HA	5.8
	HN	36	HIS	HB2	5.2
	HN	36	HIS	HD2	6
	HN	37	GLY	HN	4.4
	HN	40	LEU	QD1	7
	HN	93	HEM	QM3	7
	HA	35	CYSS	HB2	4
	HA	35	CYSS	HB3	4.1
	HA	36	HIS	HN	5.2
	HA	37	GLY	HN	6
	HA	44	SER	HN	4.9
	HA	45	ALA	QB	7
	HB2	36	HIS	HN	5.4
	HB2	36	HIS	HD2	6
	HB2	45	ALA	QB	5
	HB2	93	HEM	HT4A	4.7
	HB2	93	HEM	QT4	5.7
	HB2	93	HEM	HBM	5.2
	HB2	93	HEM	QM5	4.9
	HB3	36	HIS	HN	4.5
	HB3	44	SER	HB2	6
	HB3	44	SER	HB3	5.2
	HB3	45	ALA	QB	5.7
	HB3	93	HEM	QM3	7
	HB3	93	HEM	HT4A	5.1
	HB3	93	HEM	HBM	5.8
36 HIS					
	HN	36	HIS	HA	4.4
	HN	36	HIS	HB2	4.8
	HN	36	HIS	HB3	4.3
	HN	36	HIS	HD1	6
	HN	36	HIS	HD2	6
	HN	37	GLY	HN	4.4
	HN	40	LEU	QD1	7
	HN	45	ALA	QB	7
	HN	93	HEM	QM3	7
	HA	36	HIS	HB2	4.1
	HA	36	HIS	HB3	4.9
	HA	36	HIS	HD1	5.1
	HA	37	GLY	HN	5.1
	HA	37	GLY	HA2	6
	HA	44	SER	HN	5.6
	HA	45	ALA	QB	5.6
	HA	48	ILE	QG2	7
	HA	48	ILE	HG12	5.3
	HB2	36	HIS	HD1	5.8

	HB2	36	HIS	HD2	6
	HB2	37	GLY	HN	4.9
	HB2	40	LEU	HA	4.7
	HB2	40	LEU	HG	4.9
	HB2	40	LEU	QD2	7
	HB2	45	ALA	QB	7
	HB2	48	ILE	QG2	7
	HB2	48	ILE	HG12	5.3
	HB2	48	ILE	HG13	4.7
	HB3	36	HIS	HD1	6
	HB3	37	GLY	HN	5.4
	HB3	40	LEU	HA	4.9
	HB3	40	LEU	HB3	4.7
	HB3	40	LEU	HG	6
	HB3	40	LEU	QD1	6.7
	HB3	40	LEU	QD2	7
	HB3	45	ALA	QB	7
	HB3	48	ILE	HG12	5.3
	HB3	48	ILE	HG13	5.5
	HB3	48	ILE	QD1	6.9
	HD1	36	HIS	HD2	6
	HD1	36	HIS	HE1	4.5
	HD1	45	ALA	QB	6.1
	HD1	46	PRO	HD3	6
	HD1	47	ALA	HA	6
	HD1	48	ILE	HN	6
	HD1	48	ILE	QG2	5.8
	HD1	48	ILE	HG12	5.8
	HD1	48	ILE	HG13	4.9
	HD1	48	ILE	QD1	7
	HD2	45	ALA	QB	6.8
	HD2	48	ILE	QG2	7
	HD2	48	ILE	HG12	4.8
	HD2	48	ILE	HG13	6
	HD2	93	HEM	HT2A	5.9
	HD2	93	HEM	HAM	5.7
	HD2	93	HEM	QM3	7
	HE1	45	ALA	HA	6
	HE1	45	ALA	QB	5.4
	HE1	46	PRO	HG3	4.4
	HE1	46	PRO	HD2	5.3
	HE1	46	PRO	HD3	4.5
	HE1	48	ILE	QG2	5.4
	HE1	48	ILE	HG12	5.7
	HE1	48	ILE	HG13	5.4
	HE1	93	HEM	HBP73	6
	HE1	93	HEM	HBP74	6
	HE1	93	HEM	HGM	4.7
37 GLY					
	HN	37	GLY	HA1	4.4
	HN	37	GLY	HA2	3.4
	HN	38	GLY	HN	5.6

	HN	40	LEU	QD1	7
	HN	43	ALA	QB	6.1
	HA1	38	GLY	HN	4.1
	HA1	39	ASP-	HN	6
	HA1	40	LEU	HN	5.4
	HA1	43	ALA	QB	5.6
	HA2	38	GLY	HN	3.7
	HA2	39	ASP-	HN	5.7
	HA2	40	LEU	HN	4.5
	HA2	41	THR	HN	6
	HA2	42	GLY	HN	5.1
	HA2	43	ALA	QB	5.5
38 GLY					
	HN	38	GLY	HA1	3.6
	HN	38	GLY	HA2	4
	HN	39	ASP-	HN	4.4
	HN	40	LEU	HN	5
	HA1	39	ASP-	HN	4.9
	HA1	40	LEU	HN	4.7
	HA2	39	ASP-	HN	4.8
	HA2	40	LEU	HN	5.8
39 ASP-					
	HN	39	ASP-	HA	4.8
	HN	39	ASP-	HB2	5
	HN	39	ASP-	HB3	4.6
	HN	40	LEU	HA	5
	HN	40	LEU	QD1	7
	HN	41	THR	QG2	7
	HA	39	ASP-	HB2	4.7
	HA	39	ASP-	HB3	3.9
	HA	40	LEU	HN	4.5
	HA	41	THR	HN	6
	HB2	40	LEU	HN	5.7
	HB2	41	THR	HN	6
	HB2	41	THR	QG2	7
	HB3	41	THR	HN	5.8
	HB3	41	THR	HB	6
40 LEU					
	HN	40	LEU	HA	3.6
	HN	40	LEU	HB2	4.5
	HN	40	LEU	HB3	5
	HN	40	LEU	QD1	4.9
	HN	40	LEU	QD2	6.8
	HA	40	LEU	HB2	5
	HA	40	LEU	HB3	4.1
	HA	40	LEU	HG	5
	HA	40	LEU	QD1	4.3
	HA	40	LEU	QD2	6.8
	HA	41	THR	HN	4.5
	HA	42	GLY	HN	4.8
	HA	48	ILE	QG2	6.7
	HA	48	ILE	HG12	6

	HA	48	ILE	HG13	5.9
	HA	48	ILE	QD1	7
	HB2	40	LEU	HG	4.6
	HB2	40	LEU	QD1	4.4
	HB2	41	THR	HN	5.7
	HB2	48	ILE	HG12	6
	HB2	48	ILE	HG13	5.4
	HB2	48	ILE	QD1	6.7
	HB2	49	ASP-	HA	6
	HB2	49	ASP-	HB3	5.8
	HB3	40	LEU	HG	4.8
	HB3	40	LEU	QD1	4.5
	HB3	41	THR	HN	6
	HB3	48	ILE	HN	5.9
	HB3	48	ILE	HB	5.2
	HB3	48	ILE	QG2	7
	HB3	48	ILE	HG12	5.3
	HB3	48	ILE	HG13	4.6
	HB3	48	ILE	QD1	5.5
	HB3	49	ASP-	HN	5.5
	HB3	49	ASP-	HA	4.9
	HB3	49	ASP-	HB2	6
	HB3	49	ASP-	HB3	5.1
	HG	40	LEU	QD1	5.9
	HG	40	LEU	QD2	4.4
	HG	48	ILE	HG12	5.5
	QD1	41	THR	HN	7
	QD1	42	GLY	HN	7
	QD1	48	ILE	HN	7
	QD1	48	ILE	HG12	5.3
	QD1	48	ILE	HG13	6.5
	QD1	48	ILE	QD1	7
	QD1	49	ASP-	HN	7
	QD1	87	TRP	HZ3	7
	QD1	87	TRP	HH2	7
	QD1	88	LEU	QD2	7.1
	QD2	48	ILE	HB	5.6
	QD2	48	ILE	QG2	8
	QD2	48	ILE	HG12	6.2
	QD2	48	ILE	HG13	6.8
	QD2	48	ILE	QD1	6.2
	QD2	87	TRP	HZ3	5.5
	QD2	87	TRP	HZ2	7
	QD2	87	TRP	HH2	5.6
	QD2	88	LEU	QD1	7.1
	QD2	88	LEU	QD2	6.9
41 THR	HN	41	THR	HA	4.5
	HN	41	THR	HB	5.1
	HN	41	THR	QG2	4.5
	HN	42	GLY	HN	3.8
	HA	41	THR	HB	4.3

	HA	41	THR	QG2	4.1
	HA	42	GLY	HN	4.2
	HA	47	ALA	HA	3.7
	HA	47	ALA	QB	5.4
	HA	49	ASP-	HB2	5.4
	HA	49	ASP-	HB3	5.6
	HB	41	THR	QG2	4
	HB	42	GLY	HN	6
	QG2	42	GLY	HN	7
42 GLY					
	HN	42	GLY	HA1	3.9
	HN	42	GLY	HA2	4.3
	HN	43	ALA	HN	3.9
	HN	47	ALA	HA	3.7
	HN	47	ALA	QB	7
	HA1	43	ALA	HN	3.5
	HA1	45	ALA	HN	4.4
	HA1	46	PRO	HA	5.6
	HA1	47	ALA	HN	5.2
	HA1	47	ALA	HA	3.1
	HA1	47	ALA	QB	7
	HA2	46	PRO	HA	5.1
	HA2	47	ALA	HA	4.6
	HA2	47	ALA	QB	5.9
43 ALA					
	HN	43	ALA	HA	3.6
	HN	43	ALA	QB	4.1
	HN	44	SER	HN	4.3
	HN	45	ALA	HN	3.8
	HN	45	ALA	QB	5.7
	HA	43	ALA	QB	3.4
	HA	44	SER	HN	4.8
	QB	44	SER	HN	3.4
	QB	44	SER	HA	6.5
	QB	45	ALA	HN	4.8
44 SER					
	HN	44	SER	HA	4.7
	HN	44	SER	HB2	4.7
	HN	44	SER	HB3	4.8
	HN	45	ALA	HN	3.8
	HN	45	ALA	QB	5.5
	HA	44	SER	HB2	4.3
	HA	44	SER	HB3	4.4
	HA	45	ALA	HN	5.3
	HB2	45	ALA	HN	6
	HB3	45	ALA	HN	5.7
45 ALA					
	HN	45	ALA	HA	4.4
	HN	45	ALA	QB	3.5
	HA	45	ALA	QB	3.4
	HA	46	PRO	HD2	4
	HA	46	PRO	HD3	4.3

	HA	93	HEM	QM5	6.6
	HA	93	HEM	HGM	6
	QB	46	PRO	HB2	7
	QB	46	PRO	HB3	7
	QB	46	PRO	HG3	7
	QB	46	PRO	HD2	5.9
	QB	46	PRO	HD3	4.9
	QB	48	ILE	QG2	8
	QB	93	HEM	HT4A	6.8
	QB	93	HEM	HBM	5.7
	QB	93	HEM	QM5	5.7
	QB	93	HEM	HGM	7
	QB	93	HEM	HAP62	7
46 PRO					
	HA	46	PRO	HB2	3.6
	HA	46	PRO	HB3	4.6
	HA	46	PRO	HG2	4.2
	HA	46	PRO	HG3	5.2
	HA	46	PRO	HD2	5.1
	HA	46	PRO	HD3	5.3
	HA	47	ALA	HN	3.5
	HA	47	ALA	QB	5.3
	HB2	46	PRO	HG2	2.7
	HB2	46	PRO	HG3	3.6
	HB2	46	PRO	HD2	6
	HB2	47	ALA	HN	4.5
	HB2	47	ALA	QB	6.5
	HB2	93	HEM	HAP62	6
	HB3	46	PRO	HG2	2.7
	HB3	46	PRO	HG3	4.3
	HB3	46	PRO	HD2	5.9
	HB3	46	PRO	HD3	5.2
	HB3	47	ALA	HN	5
	HB3	93	HEM	HBP73	6
	HB3	93	HEM	HGM	6
	HB3	93	HEM	HAP62	6
	HG2	46	PRO	HD2	3.5
	HG2	46	PRO	HD3	3.4
	HG2	93	HEM	HGM	4.6
	HG3	46	PRO	HD2	6
	HG3	46	PRO	HD3	4.3
	HG3	47	ALA	HN	4.4
	HG3	48	ILE	QG2	7
	HG3	93	HEM	HBP73	6
	HG3	93	HEM	QM8	7
	HD3	48	ILE	QG2	7
	HD3	93	HEM	QM5	7
	HD3	93	HEM	HGM	6
	HD3	93	HEM	HAP62	5.2
47 ALA					
	HN	47	ALA	HA	4.2
	HN	47	ALA	QB	3.4

	HN	47	ALA	HB2	4.6
	HN	48	ILE	QG2	7
	HA	47	ALA	QB	3.7
	HA	48	ILE	HN	3.9
	HA	48	ILE	QG2	7
	HA	48	ILE	HG12	6
	HA	48	ILE	HG13	5.6
	HA	49	ASP-	HN	4.4
	QB	48	ILE	HN	4
	QB	48	ILE	QG2	8
	QB	49	ASP-	HN	4.3
	QB	49	ASP-	HB3	5.2
	QB	50	LYS+	HN	5.2
	QB	50	LYS+	HB2	5.2
48 ILE	HN	48	ILE	HA	4.3
	HN	48	ILE	HB	5.5
	HN	48	ILE	QG2	5.5
	HN	48	ILE	HG12	6
	HN	48	ILE	HG13	4.8
	HN	48	ILE	QD1	5.6
	HN	49	ASP-	HN	3.5
	HN	49	ASP-	HA	6
	HN	49	ASP-	HB2	6
	HN	49	ASP-	HB3	6
	HA	48	ILE	HB	3.5
	HA	48	ILE	QG2	4.2
	HA	48	ILE	HG12	6
	HA	48	ILE	HG13	6
	HA	48	ILE	QD1	7
	HA	49	ASP-	HN	4.4
	HA	50	LYS+	HN	4.9
	HA	51	ALA	HN	5.1
	HA	51	ALA	HA	4.5
	HA	51	ALA	QB	4.1
	HA	93	HEM	QM8	7
	HB	48	ILE	QG2	4.1
	HB	48	ILE	HG12	4.4
	HB	48	ILE	HG13	4.8
	HB	48	ILE	QD1	4.7
	HB	49	ASP-	HN	5.3
	HB	51	ALA	HN	5.2
	HB	51	ALA	QB	4.4
	HB	93	HEM	QM8	6.9
	HB	93	HEM	HDM	5.6
	QG2	48	ILE	HG12	4.1
	QG2	48	ILE	HG13	4.3
	QG2	48	ILE	QD1	6
	QG2	49	ASP-	HN	7
	QG2	51	ALA	HN	7
	QG2	51	ALA	QB	7.1
	QG2	88	LEU	HG	7

	QG2	88	LEU	QD1	8
	QG2	93	HEM	HAP71	7
	QG2	93	HEM	HAP72	7
	QG2	93	HEM	HBP73	6.4
	QG2	93	HEM	HBP74	4.8
	QG2	93	HEM	HDM	6.8
	QG2	93	HEM	HGM	7
	HG12	48	ILE	QD1	4.3
	HG12	49	ASP-	HN	6
	HG12	51	ALA	QB	7
	HG12	84	VAL	QG2	5.9
	HG12	88	LEU	QD1	5.6
	HG12	93	HEM	HBP74	5.3
	HG12	93	HEM	HDM	4.6
	HG12	93	HEM	QM1	5.7
	HG13	48	ILE	QD1	3.6
	HG13	49	ASP-	HN	5.7
	HG13	88	LEU	QD1	7
	HG13	93	HEM	HBP74	6
	QD1	88	LEU	QD1	7.9
	QD1	88	LEU	QD2	8
	QD1	93	HEM	QM1	7
49 ASP-					
	HN	49	ASP-	HA	4.3
	HN	49	ASP-	HB2	4.8
	HN	49	ASP-	HB3	4.1
	HN	50	LYS+	HN	3.9
	HN	51	ALA	HN	5.8
	HA	49	ASP-	HB2	3.3
	HA	49	ASP-	HB3	3.4
	HA	50	LYS+	HN	5.2
	HA	51	ALA	HN	5.6
	HA	88	LEU	QD1	7
	HA	88	LEU	QD2	7
	HB2	50	LYS+	HN	6
	HB3	50	LYS+	HN	5.5
	HB3	51	ALA	HN	6
50 LYS+					
	HN	50	LYS+	HA	4.1
	HN	50	LYS+	HB2	4.5
	HN	50	LYS+	HB3	4.2
	HN	50	LYS+	HG2	5.6
	HN	50	LYS+	HG3	6
	HN	50	LYS+	HD2	6
	HN	50	LYS+	HD3	6
	HN	50	LYS+	QE	7
	HN	51	ALA	HN	3.7
	HN	51	ALA	QB	4.9
	HA	50	LYS+	HB2	3.5
	HA	50	LYS+	HB3	4.7
	HA	50	LYS+	HG2	5.7
	HA	50	LYS+	HG3	5.3

	HA	50	LYS+	HD3	6
	HA	51	ALA	HN	4.4
	HA	53	ALA	QB	5.9
	HB2	50	LYS+	HG2	4.8
	HB2	50	LYS+	HG3	4.8
	HB2	50	LYS+	QE	7
	HB2	51	ALA	HN	4.6
	HB3	50	LYS+	QE	7
	HB3	51	ALA	HN	4.9
	HG2	50	LYS+	QE	7
	HG2	51	ALA	HN	5.9
	HG3	50	LYS+	QE	7
	HG3	51	ALA	HN	6
	HG3	53	ALA	QB	7
	HD2	50	LYS+	QE	7
	HD3	50	LYS+	QE	7
51 ALA					
	HN	51	ALA	HA	3.9
	HN	51	ALA	QB	3.4
	HN	52	GLY	HN	4.4
	HN	53	ALA	HN	6
	HA	51	ALA	QB	3.4
	HA	52	GLY	HN	4.4
	HA	53	ALA	HN	5.1
	HA	54	ASN	HN	5.2
	HA	54	ASN	HB2	5.3
	HA	54	ASN	HB3	6
	HA	54	ASN	HD21	6
	HA	54	ASN	HD22	6
	HA	55	TYR	HN	6
	HA	55	TYR	QD	7.8
	HA	55	TYR	QE	8
	HA	60	ILE	QG1	6.5
	QB	52	GLY	HN	4.3
	QB	54	ASN	HN	6.7
	QB	55	TYR	HB3	6.6
	QB	55	TYR	QD	8.4
	QB	55	TYR	QE	9
	QB	60	ILE	QG2	6.4
	QB	60	ILE	QG1	8
	QB	60	ILE	QD1	6.9
	QB	88	LEU	HB2	6.1
	QB	88	LEU	HB3	5
	QB	88	LEU	QD1	7.1
	QB	88	LEU	QD2	6.6
	QB	93	HEM	QM8	5.7
52 GLY					
	HN	52	GLY	HA1	4
	HN	52	GLY	HA2	3.7
	HN	53	ALA	HN	4
	HN	53	ALA	HA	6
	HN	53	ALA	QB	5.6

	HN	54	ASN	HN	5.2
	HN	88	LEU	HB3	5.3
	HN	89	ALA	HA	4.2
	HN	91	LYS+	HN	4.9
	HN	91	LYS+	HB2	5
	HN	92	LYS+	HN	6
	HA1	53	ALA	HN	5.1
	HA1	54	ASN	HN	5.5
	HA1	55	TYR	HN	4.7
	HA1	55	TYR	HB3	6
	HA1	60	ILE	QD1	5.3
	HA1	89	ALA	HA	3.8
	HA1	89	ALA	QB	6.9
	HA2	53	ALA	HN	5
	HA2	54	ASN	HN	5.3
	HA2	55	TYR	HN	5.6
	HA2	89	ALA	HA	3.1
	HA2	92	LYS+	QE	7
53 ALA					
	HN	53	ALA	HA	4.1
	HN	53	ALA	QB	3.4
	HN	54	ASN	HN	3.8
	HN	54	ASN	HB2	6
	HN	55	TYR	HN	3.9
	HN	91	LYS+	HB3	6
	HN	92	LYS+	HA	3.6
	HN	92	LYS+	HB2	6
	HN	92	LYS+	QG	5.7
	HA	53	ALA	QB	3.5
	HA	54	ASN	HN	4.8
	HA	55	TYR	HN	5.5
	HA	92	LYS+	HA	6
	HA	92	LYS+	QD	7
	HA	92	LYS+	QE	7
	QB	54	ASN	HN	4
	QB	54	ASN	HA	6.5
	QB	54	ASN	HD21	7
	QB	54	ASN	HD22	7
	QB	55	TYR	HN	7
	QB	92	LYS+	HA	5.7
	QB	92	LYS+	QG	6.6
	QB	92	LYS+	QD	6.5
54 ASN					
	HN	54	ASN	HA	4.6
	HN	54	ASN	HB2	3.9
	HN	54	ASN	HB3	4.5
	HN	55	TYR	HN	3.5
	HN	55	TYR	HA	6
	HA	54	ASN	HB2	4.8
	HA	54	ASN	HB3	4.5
	HA	55	TYR	HN	5.5
	HB2	54	ASN	HD21	5.7

	HB2	54	ASN	HD22	6
	HB2	55	TYR	HN	5
	HB2	55	TYR	QD	6.7
	HB3	54	ASN	HD21	6
	HB3	54	ASN	HD22	6
	HB3	55	TYR	HN	5.8
	HB3	55	TYR	QD	7.4
	HB3	55	TYR	QE	8
	HD21	55	TYR	QE	6.6
	HD22	55	TYR	QD	7.4
	HD22	55	TYR	QE	8
55 TYR					
	HN	55	TYR	HA	4.5
	HN	55	TYR	HB2	5.2
	HN	55	TYR	HB3	4.3
	HN	55	TYR	QD	8
	HN	55	TYR	QE	7
	HN	56	SER	HN	6
	HA	55	TYR	HB2	4.5
	HA	55	TYR	HB3	4.4
	HA	55	TYR	QD	6.5
	HA	55	TYR	QE	6.6
	HA	56	SER	HN	3.4
	HA	59	GLU-	HB2	5
	HA	59	GLU-	HB3	4.8
	HA	59	GLU-	HG2	6
	HB2	55	TYR	QD	7.3
	HB2	55	TYR	QE	8
	HB2	56	SER	HN	4.5
	HB2	59	GLU-	HB2	4.5
	HB2	59	GLU-	HB3	4.3
	HB2	60	ILE	HN	5.8
	HB2	60	ILE	QG1	6.7
	HB2	60	ILE	QD1	7
	HB3	55	TYR	QD	7.4
	HB3	55	TYR	QE	8
	HB3	56	SER	HN	4.5
	HB3	59	GLU-	HN	4.7
	HB3	59	GLU-	HB2	3.7
	HB3	59	GLU-	HB3	4.3
	HB3	59	GLU-	HG2	4.9
	HB3	59	GLU-	HG3	5
	HB3	60	ILE	HN	5.1
	HB3	60	ILE	QD1	7
	QD	55	TYR	QE	9.1
	QD	56	SER	HN	8
	QD	59	GLU-	HB2	6.6
	QD	59	GLU-	HB3	7.5
	QD	60	ILE	QD1	9
	QD	63	ILE	HG13	8
	QD	93	HEM	HAP72	8
	QD	93	HEM	HBP74	8

	QD	93	HEM	QM8	9
	QE	59	GLU-	HB2	8
	QE	59	GLU-	HG2	8
	QE	63	ILE	HG13	7.5
	QE	63	ILE	QD1	9
	QE	68	GLN	HE22	7.5
	QE	93	HEM	HAP71	8
	QE	93	HEM	HAP72	7.3
	QE	93	HEM	HBP74	7.2
56 SER					
	HN	56	SER	HA	4.5
	HN	56	SER	HB2	4.9
	HN	56	SER	HB3	4.3
	HN	57	GLU-	HN	4.6
	HN	58	GLU-	HN	6
	HN	59	GLU-	HN	5.2
	HN	59	GLU-	HB2	3.8
	HN	59	GLU-	HB3	4
	HN	59	GLU-	HG2	6
	HN	59	GLU-	HG3	6
	HN	60	ILE	HN	5.7
	HA	56	SER	HB3	5
	HA	57	GLU-	HN	3.6
	HA	57	GLU-	QG	7
	HA	58	GLU-	HN	5.3
	HA	59	GLU-	HN	6
	HA	89	ALA	QB	7
	HB2	57	GLU-	HN	3.9
	HB2	58	GLU-	HN	4.7
	HB2	58	GLU-	HB2	6
	HB2	59	GLU-	HN	5.9
	HB2	59	GLU-	HB2	6
	HB3	57	GLU-	HN	4.9
	HB3	57	GLU-	QG	6.9
	HB3	58	GLU-	HN	5.5
	HB3	58	GLU-	HB2	5.9
	HB3	58	GLU-	HG2	6
	HB3	59	GLU-	HN	4.9
	HB3	59	GLU-	HB2	5.2
57 GLU-					
	HN	57	GLU-	HA	4.3
	HN	57	GLU-	HB2	3.6
	HN	57	GLU-	HB3	3.8
	HN	57	GLU-	QG	6.9
	HN	58	GLU-	HN	4.4
	HN	59	GLU-	HN	6
	HN	89	ALA	QB	5.9
	HA	57	GLU-	HB2	3.7
	HA	57	GLU-	HB3	5.3
	HA	57	GLU-	QG	6.6
	HA	58	GLU-	HN	4.5
	HA	60	ILE	HN	4.8

	HA	60	ILE	HB	3.5
	HA	60	ILE	QG2	5.5
	HA	60	ILE	QG1	6
	HA	85	ALA	QB	5.4
	HA	89	ALA	QB	5.1
	HB2	58	GLU-	HN	4.3
	HB2	85	ALA	QB	5.4
	HB2	86	ALA	HA	4.7
	HB2	86	ALA	QB	6.5
	HB2	89	ALA	QB	5
	HB3	58	GLU-	HN	4.5
	HB3	86	ALA	HA	5.1
	HB3	86	ALA	QB	6.7
	HB3	89	ALA	HN	5.1
	HB3	90	GLU-	HB2	5.5
	QG	58	GLU-	HA	6.4
	QG	58	GLU-	HG2	6.4
	QG	58	GLU-	HG3	6
	QG	86	ALA	HA	6.7
58 GLU-					
	HN	58	GLU-	HA	4.3
	HN	58	GLU-	HB2	3.7
	HN	58	GLU-	HB3	3.6
	HN	58	GLU-	HG2	6
	HN	58	GLU-	HG3	6
	HN	59	GLU-	HN	4.2
	HN	60	ILE	HN	5.4
	HA	58	GLU-	HB2	4
	HA	58	GLU-	HB3	3.6
	HA	58	GLU-	HG2	6
	HA	58	GLU-	HG3	4.7
	HA	59	GLU-	HN	5.2
	HA	61	LEU	HN	4.3
	HA	61	LEU	HB2	4.3
	HA	61	LEU	HB3	3.8
	HA	61	LEU	QD1	7
	HA	61	LEU	QD2	6.8
	HA	62	ASP-	HN	5.2
	HB2	59	GLU-	HN	4.3
	HB2	59	GLU-	HG3	4
	HB3	59	GLU-	HN	4.4
	HG2	59	GLU-	HN	5.9
	HG2	59	GLU-	HA	6
	HG2	59	GLU-	HB2	4
	HG3	59	GLU-	HG2	3.2
	HG3	59	GLU-	HG3	3.9
59 GLU-					
	HN	59	GLU-	HA	4.9
	HN	59	GLU-	HB2	4.5
	HN	59	GLU-	HB3	3.9
	HN	59	GLU-	HG2	5.4
	HN	59	GLU-	HG3	5.7

	HN	60	ILE	HN	4.3
	HN	60	ILE	HA	5.4
	HN	60	ILE	QG1	6.4
	HN	61	LEU	HN	4.3
	HA	59	GLU-	HB2	5.9
	HA	59	GLU-	HB3	4.4
	HA	59	GLU-	HG2	5.7
	HA	59	GLU-	HG3	5.2
	HA	60	ILE	HN	5.6
	HA	61	LEU	HN	6
	HA	62	ASP-	HN	4.5
	HA	62	ASP-	HB2	5
	HA	62	ASP-	HB3	4.6
	HA	63	ILE	HN	6
	HB2	60	ILE	HN	3.6
	HB2	60	ILE	HA	4.7
	HB2	60	ILE	QG1	6.4
	HB2	60	ILE	QD1	4.9
	HB2	63	ILE	HG13	6
	HB3	59	GLU-	HG2	5.7
	HB3	59	GLU-	HG3	5.3
	HB3	60	ILE	HN	4.6
	HG3	60	ILE	HN	6
60 ILE					
	HN	60	ILE	HA	4.7
	HN	60	ILE	HB	3.4
	HN	60	ILE	QG2	6.1
	HN	60	ILE	QG1	7
	HN	60	ILE	QD1	5.4
	HN	62	ASP-	HN	4.1
	HA	60	ILE	HB	4.7
	HA	60	ILE	QG1	6.2
	HA	60	ILE	QD1	6.3
	HA	61	LEU	HN	4.9
	HA	62	ASP-	HN	6
	HA	63	ILE	HN	4.6
	HA	63	ILE	HB	4.1
	HA	63	ILE	QG2	7
	HA	63	ILE	HG13	4.4
	HA	64	ILE	HN	4.5
	HA	93	HEM	QM8	6.6
	HB	60	ILE	QG1	5.9
	HB	60	ILE	QD1	5.1
	HB	61	LEU	HN	3.9
	HB	63	ILE	QG2	7
	HB	85	ALA	HA	5.1
	HB	85	ALA	QB	4.7
	QG2	61	LEU	HN	7
	QG2	61	LEU	HA	7
	QG2	64	ILE	HN	7
	QG2	64	ILE	HG13	6.6
	QG2	64	ILE	QD1	6.6

	QG2	85	ALA	HA	7
	QG2	85	ALA	QB	6.6
	QG2	88	LEU	HB2	5.2
	QG2	88	LEU	HB3	5.6
	QG2	88	LEU	HG	7
	QG2	93	HEM	QM8	7
	QG2	93	HEM	HDM	7
	QG2	93	HEM	QM1	6
	QG1	60	ILE	QD1	6.4
	QG1	61	LEU	HN	6.2
	QG1	63	ILE	QG2	8
	QG1	85	ALA	HA	5.3
	QG1	93	HEM	QM8	7.1
	QD1	88	LEU	HB2	6.2
	QD1	88	LEU	HB3	7
	QD1	93	HEM	QM8	7
61 LEU					
	HN	61	LEU	HA	4.3
	HN	61	LEU	HB2	3.5
	HN	61	LEU	HB3	3.7
	HN	61	LEU	HG	6
	HN	61	LEU	QD1	6.2
	HN	61	LEU	QD2	6.5
	HN	62	ASP-	HN	4.5
	HN	63	ILE	HN	5.9
	HN	85	ALA	HA	5.6
	HN	85	ALA	QB	5.4
	HA	61	LEU	HB2	4
	HA	61	LEU	HB3	3.7
	HA	61	LEU	HG	5.2
	HA	61	LEU	QD1	4.2
	HA	61	LEU	QD2	7
	HA	62	ASP-	HN	5.4
	HA	63	ILE	HN	6
	HA	64	ILE	HN	4.3
	HA	64	ILE	QG2	7
	HA	64	ILE	HG13	6
	HB2	61	LEU	HG	4.4
	HB2	62	ASP-	HN	4.6
	HB2	63	ILE	HN	5.6
	HB2	64	ILE	HN	6
	HB2	82	GLU-	HA	5.2
	HB2	85	ALA	QB	4.6
	HB3	61	LEU	HG	4.8
	HB3	61	LEU	QD1	5.3
	HB3	61	LEU	QD2	4.4
	HB3	62	ASP-	HN	3.8
	HG	61	LEU	QD1	3.7
	HG	61	LEU	QD2	4.1
	HG	62	ASP-	HN	5.6
	HG	62	ASP-	HA	3.9
	HG	65	LEU	HG	3.8

	HG	65	LEU	QD1	5.6
	HG	81	ALA	QB	6.9
	QD1	62	ASP-	HN	7
	QD1	65	LEU	QD1	7.2
	QD1	81	ALA	QB	6
	QD1	82	GLU-	HN	6.5
	QD1	82	GLU-	HA	5.4
	QD1	82	GLU-	HB2	6.9
	QD1	82	GLU-	HB3	7
	QD1	82	GLU-	HG2	6.3
	QD1	82	GLU-	HG3	5.7
	QD1	85	ALA	HN	7
	QD1	85	ALA	QB	6.1
	QD2	62	ASP-	HA	6
	QD2	81	ALA	QB	6.3
	QD2	82	GLU-	HA	6.4
	QD2	82	GLU-	HB2	6.8
	QD2	82	GLU-	HG3	4.9
62 ASP-					
	HN	62	ASP-	HA	4.2
	HN	62	ASP-	HB2	3.5
	HN	62	ASP-	HB3	3.7
	HN	63	ILE	HN	3.7
	HA	62	ASP-	HB2	3.9
	HA	62	ASP-	HB3	4
	HA	63	ILE	HN	5.3
	HA	64	ILE	HN	4.6
	HA	65	LEU	HN	4.7
	HA	65	LEU	HB2	4.6
	HA	65	LEU	HB3	3.5
	HA	65	LEU	HG	5.1
	HA	65	LEU	QD1	7
	HA	66	ASN	HN	5.8
	HA	66	ASN	HD21	5.6
	HA	66	ASN	HD22	5.3
	HB2	63	ILE	HN	4.7
	HB2	63	ILE	HB	6
	HB3	66	ASN	HD22	6
63 ILE					
	HN	63	ILE	HA	3.8
	HN	63	ILE	HB	3.3
	HN	63	ILE	QG2	5.8
	HN	63	ILE	HG12	4.5
	HN	63	ILE	HG13	5.5
	HN	63	ILE	QD1	5.3
	HN	64	ILE	HN	3.9
	HN	64	ILE	HG12	4.1
	HN	64	ILE	QD1	7
	HN	65	LEU	HN	5.8
	HN	65	LEU	HG	6
	HA	63	ILE	HB	3.9
	HA	63	ILE	QG2	4.7

HA	63	ILE	HG12	3.5
HA	63	ILE	HG13	6
HA	63	ILE	QD1	4.6
HA	64	ILE	HN	4.5
HA	65	LEU	HN	6
HA	66	ASN	HN	5
HA	66	ASN	HB2	3.2
HA	66	ASN	HB3	4.1
HA	66	ASN	HD21	6
HA	67	GLY	HN	4.5
HA	68	GLN	HB2	6
HA	71	MET	QE	7
HB	63	ILE	QG2	4.3
HB	63	ILE	HG13	4.2
HB	63	ILE	QD1	3.7
HB	64	ILE	HN	4
QG2	63	ILE	HG12	4.4
QG2	63	ILE	HG13	4.2
QG2	63	ILE	QD1	5.7
QG2	64	ILE	HN	6.8
QG2	64	ILE	HA	7
QG2	64	ILE	QG2	8
QG2	64	ILE	HG13	7
QG2	64	ILE	QD1	8
QG2	65	LEU	HN	7
QG2	68	GLN	HB2	6.4
QG2	68	GLN	HB3	6.3
QG2	68	GLN	HE21	7
QG2	71	MET	QE	6.2
QG2	93	HEM	HAP71	7
QG2	93	HEM	HAP72	7
QG2	93	HEM	QM8	6.3
QG2	93	HEM	HDM	7
QG2	93	HEM	HGM	7
HG12	63	ILE	QD1	3.8
HG13	63	ILE	QD1	4
HG13	64	ILE	HN	6
HG13	68	GLN	HB2	5.7
HG13	68	GLN	HE21	6
HG13	68	GLN	HE22	5.4
HG13	93	HEM	HAP71	4.7
HG13	93	HEM	HAP72	4.5
HG13	93	HEM	QM8	5.7
HG13	93	HEM	HGM	6
QD1	64	ILE	HN	7
QD1	66	ASN	HB2	7
QD1	66	ASN	HB3	7
QD1	68	GLN	HB2	6.4
QD1	68	GLN	HB3	7
QD1	68	GLN	HG2	7
QD1	93	HEM	QM8	7

64 ILE

HN	64	ILE	HA	4.3
HN	64	ILE	HB	3.6
HN	64	ILE	QG2	5.6
HN	64	ILE	HG12	5.1
HN	64	ILE	HG13	5.1
HN	64	ILE	QD1	5
HN	65	LEU	HN	4.1
HN	65	LEU	HB3	5.5
HN	65	LEU	HG	5.6
HN	66	ASN	HN	5.1
HN	71	MET	QE	7
HA	64	ILE	HB	4.7
HA	64	ILE	QG2	4.3
HA	64	ILE	HG12	3.9
HA	64	ILE	HG13	4.9
HA	64	ILE	QD1	5.2
HA	65	LEU	HN	6
HA	66	ASN	HN	4.5
HA	71	MET	QE	5.1
HB	64	ILE	QG2	4.4
HB	64	ILE	HG13	4.9
HB	64	ILE	QD1	4.1
HB	65	LEU	HN	4.2
HB	65	LEU	HG	4.7
HB	71	MET	QE	7
QG2	64	ILE	HG12	4.5
QG2	64	ILE	HG13	3.7
QG2	64	ILE	QD1	4.9
QG2	65	LEU	HN	7
QG2	65	LEU	HA	6.9
QG2	65	LEU	HG	7
QG2	71	MET	QE	7.7
QG2	75	ILE	HN	7
QG2	75	ILE	HB	7
QG2	75	ILE	QG2	8
QG2	76	ALA	HN	5.8
QG2	76	ALA	QB	5.7
QG2	81	ALA	HA	6.5
QG2	81	ALA	QB	6.5
QG2	84	VAL	HB	7
QG2	84	VAL	QG1	8
QG2	93	HEM	HDM	7
QG2	93	HEM	QM1	7
QG2	93	HEM	QT2	5.2
HG21	93	HEM	QM1	7
HG12	64	ILE	QD1	3.4
HG12	65	LEU	HN	5.4
HG12	93	HEM	HDM	4.6
HG12	93	HEM	QM1	7
HG13	64	ILE	QD1	3.4
HG13	65	LEU	HN	6
HG13	71	MET	QE	5.3

	HG13	84	VAL	QG1	6.6
	HG13	85	ALA	QB	6.9
	HG13	93	HEM	QM8	7
	HG13	93	HEM	HDM	6
	HG13	93	HEM	QM1	6.5
	HG13	93	HEM	QT2	6.1
	QD1	65	LEU	HN	7
	QD1	71	MET	QE	8
	QD1	84	VAL	HB	6
	QD1	84	VAL	QG1	5.7
	QD1	84	VAL	QG2	6.7
	QD1	85	ALA	HN	6.1
	QD1	85	ALA	HA	6.2
	QD1	93	HEM	HDM	7
	QD1	93	HEM	QM1	5.6
	QD1	93	HEM	QT2	6.1
65 LEU	HN	65	LEU	HA	4
	HN	65	LEU	HB2	3.4
	HN	65	LEU	HB3	4.4
	HN	65	LEU	HG	4.8
	HN	65	LEU	QD1	4.3
	HN	65	LEU	QD2	6.5
	HN	66	ASN	HN	4
	HN	67	GLY	HN	5.1
	HA	65	LEU	HB2	4.5
	HA	65	LEU	HB3	3.7
	HA	65	LEU	HG	3.9
	HA	65	LEU	QD1	5.1
	HA	65	LEU	QD2	6.2
	HA	66	ASN	HN	4.7
	HA	67	GLY	HN	6
	HA	73	GLY	HA1	6
	HA	74	GLY	HN	3.4
	HA	76	ALA	HN	6
	HA	81	ALA	QB	6.1
	HB2	65	LEU	HG	5.1
	HB2	66	ASN	HN	4.3
	HB2	66	ASN	HD21	6
	HB3	65	LEU	HG	4.2
	HB3	65	LEU	QD1	4.6
	HB3	65	LEU	QD2	6.3
	HB3	66	ASN	HN	4.6
	HB3	76	ALA	HN	6
	HG	65	LEU	QD1	3.6
	HG	65	LEU	QD2	4.1
	HG	66	ASN	HN	5.3
	HG	66	ASN	HD21	6
	HG	74	GLY	HN	6
	HG	76	ALA	HN	6
	HG	77	LYS+	HA	4.8
	HG	81	ALA	HN	5.3

	HG	81	ALA	QB	5.3
	QD1	66	ASN	HN	6.8
	QD1	81	ALA	QB	7.8
	QD2	74	GLY	HN	7
	QD2	74	GLY	HA1	7
	QD2	74	GLY	HA2	7
	QD2	76	ALA	HA	7
	QD2	77	LYS+	HA	7
	QD2	77	LYS+	HB3	5.6
	QD2	77	LYS+	QD	8
	QD2	78	GLY	HN	7
	QD2	81	ALA	HN	7
	QD2	81	ALA	QB	6.6
66 ASN					
	HN	66	ASN	HA	4.3
	HN	66	ASN	HB2	4.9
	HN	66	ASN	HB3	4.7
	HN	66	ASN	HD21	5.9
	HN	66	ASN	HD22	6
	HN	67	GLY	HN	3.7
	HN	67	GLY	HA1	6
	HN	67	GLY	HA2	4.7
	HA	66	ASN	HB2	4.2
	HA	66	ASN	HB3	4
	HA	66	ASN	HD22	6
	HA	67	GLY	HN	5.1
	HA	73	GLY	HA2	4.2
	HB2	66	ASN	HD21	5.3
	HB2	66	ASN	HD22	4.8
	HB2	67	GLY	HN	4.9
	HB3	66	ASN	HD21	5.8
	HB3	66	ASN	HD22	6
67 GLY					
	HN	67	GLY	HA1	4.2
	HN	67	GLY	HA2	3.8
	HN	68	GLN	HN	6
	HN	71	MET	QE	7
	HN	73	GLY	HA1	4.1
	HN	73	GLY	HA2	3.5
	HA1	68	GLN	HN	4.2
	HA1	71	MET	QE	7
	HA1	73	GLY	HN	4.6
	HA1	73	GLY	HA1	3.9
	HA1	73	GLY	HA2	4.6
	HA2	68	GLN	HN	3.9
	HA2	71	MET	HG2	6
	HA2	71	MET	QE	7
	HA2	73	GLY	HN	5.7
	HA2	73	GLY	HA1	5.3
68 GLN					
	HN	68	GLN	HA	4.7
	HN	68	GLN	HB2	5.3

	HN	68	GLN	HB3	4.9
	HN	68	GLN	HG2	6
	HN	68	GLN	HG3	6
	HN	69	GLY	HN	6
	HN	71	MET	HN	5.5
	HN	71	MET	HB2	4.9
	HN	71	MET	HB3	4.2
	HN	71	MET	HG2	6
	HN	71	MET	QE	7
	HA	68	GLN	HB2	3.9
	HA	68	GLN	HB3	4.1
	HA	68	GLN	HG2	6
	HA	68	GLN	HG3	5.7
	HA	69	GLY	HN	4
	HA	69	GLY	HA2	3.7
	HB2	68	GLN	HG2	5
	HB2	68	GLN	HE21	6
	HB2	68	GLN	HE22	6
	HB2	69	GLY	HN	6
	HB2	93	HEM	HBP74	5
	HB3	68	GLN	HE21	6
	HB3	68	GLN	HE22	6
	HG2	68	GLN	HE21	4.8
	HG2	68	GLN	HE22	5.8
	HG2	69	GLY	HA2	6
	HG2	93	HEM	HAP62	4.6
	HG2	93	HEM	HBP63	6
	HG2	93	HEM	HBP64	6
	HG3	68	GLN	HE21	6
	HG3	68	GLN	HE22	6
	HG3	69	GLY	HN	5.3
	HG3	93	HEM	HBP63	5.7
	HE21	93	HEM	HAP71	6
	HE21	93	HEM	HAP72	6
	HE21	93	HEM	HGM	6
	HE21	93	HEM	HBP63	6
	HE21	93	HEM	HBP64	6
	HE22	93	HEM	HAP71	5.5
	HE22	93	HEM	HAP72	6
	HE22	93	HEM	HBP74	6
	HE22	93	HEM	HGM	6
	HE22	93	HEM	HBP63	6
	HE22	93	HEM	HBP64	6
69 GLY					
	HN	69	GLY	HA1	3.9
	HN	69	GLY	HA2	3.6
	HN	70	GLY	HN	6
	HA1	70	GLY	HN	3.6
	HA1	93	HEM	HBP63	6
	HA2	70	GLY	HN	4.1
	HA2	71	MET	HN	6
	HA2	93	HEM	HBP63	5.8

70 GLY	HA2	93	HEM	HBP64	5.8
	HN	70	GLY	HA1	4.3
	HN	70	GLY	HA2	3.7
	HN	71	MET	HN	4.5
	HN	71	MET	HA	5.3
	HN	93	HEM	QM5	7
	HN	93	HEM	HAP61	6
	HN	93	HEM	HBP63	5.6
	HN	93	HEM	HBP64	4.8
	HA1	71	MET	HN	5.8
	HA2	71	MET	HN	5
	HA2	93	HEM	QM5	6.8
71 MET	HN	71	MET	HA	5
	HN	71	MET	HB2	4.3
	HN	71	MET	HB3	4.3
	HN	71	MET	HG2	6
	HN	93	HEM	QM5	7
	HN	93	HEM	HBP64	5.1
	HA	71	MET	HB2	4.4
	HA	71	MET	HB3	6
	HA	71	MET	QE	7
	HA	93	HEM	QT4	7
	HB2	71	MET	HG2	5.8
	HB2	71	MET	HG3	5.9
	HB2	71	MET	QE	7
	HB2	93	HEM	HBM	6
	HB2	93	HEM	QM5	7
	HB2	93	HEM	HGM	6
	HB2	93	HEM	HBP64	5.8
	HB3	71	MET	HG2	5.9
	HB3	71	MET	HG3	6
	HB3	71	MET	QE	7
	HG2	71	MET	QE	4.8
	HG2	75	ILE	QD1	7
	HG3	71	MET	QE	5.6
	HG3	75	ILE	QD1	7
	HG3	93	HEM	HBM	6
	QE	73	GLY	HA1	7
	QE	75	ILE	HN	7
	QE	75	ILE	HB	7
	QE	75	ILE	QG2	8
	QE	75	ILE	HG12	7
	QE	76	ALA	QB	8
	QE	93	HEM	QM8	7
	QE	93	HEM	HDM	7
	QE	93	HEM	QM1	7
	QE	93	HEM	HT2A	7
	QE	93	HEM	QT2	6.8
	QE	93	HEM	HAM	7
	QE	93	HEM	QM3	7

72 PRO					
HA	72	PRO	QB	3.9	
HA	72	PRO	QG	4.7	
HA	72	PRO	QD	7	
HA	73	GLY	HN	3.5	
HA	73	GLY	HA1	5.2	
HA	73	GLY	HA2	6	
QB	72	PRO	QG	6.6	
QB	73	GLY	HN	6.4	
QG	73	GLY	HN	5.5	
73 GLY					
HN	73	GLY	HA1	4.3	
HN	73	GLY	HA2	3.9	
HN	74	GLY	HN	4.3	
HA1	74	GLY	HN	3.8	
HA1	75	ILE	HN	6	
HA2	74	GLY	HN	4.2	
74 GLY					
HN	74	GLY	HA1	4.1	
HN	74	GLY	HA2	3.8	
HN	75	ILE	HN	4.5	
HN	76	ALA	HN	5.6	
HA1	75	ILE	HN	5.7	
HA1	76	ALA	HN	5.8	
HA1	77	LYS+	QE	7	
HA2	77	LYS+	QG	6.8	
HA2	77	LYS+	QD	6.8	
HA2	77	LYS+	QE	7	
75 ILE					
HN	75	ILE	HA	4.1	
HN	75	ILE	HB	3.7	
HN	75	ILE	QG2	6.3	
HN	75	ILE	HG12	5.3	
HN	75	ILE	HG13	5.7	
HN	75	ILE	QD1	6.3	
HN	76	ALA	HN	3.9	
HA	75	ILE	HB	4.6	
HA	75	ILE	QG2	4.8	
HA	75	ILE	HG12	5.5	
HA	75	ILE	HG13	5.3	
HA	75	ILE	QD1	5.7	
HA	76	ALA	HN	4.6	
HB	75	ILE	QG2	4	
HB	75	ILE	HG12	4.2	
HB	75	ILE	HG13	5.3	
HB	75	ILE	QD1	4.7	
HB	76	ALA	HN	4.2	
HB	93	HEM	HT2A	6	
HB	93	HEM	QT2	4.4	
HB	93	HEM	HAM	6	
QG2	75	ILE	HG13	5.1	
QG2	75	ILE	QD1	5.1	

	QG2	76	ALA	HN	7
	QG2	76	ALA	HA	7
	QG2	76	ALA	QB	6.6
	QG2	93	HEM	HT2A	6
	QG2	93	HEM	QT2	4.9
	QG2	93	HEM	HAM	6.2
	QG2	93	HEM	QM3	6.7
	HG12	75	ILE	QD1	4.7
	HG12	93	HEM	QM3	6.9
	HG13	75	ILE	QD1	5.4
	HG13	76	ALA	HN	6
	QD1	76	ALA	HN	7
	QD1	93	HEM	HT2A	6.8
	QD1	93	HEM	HAM	6.3
	QD1	93	HEM	QM3	5.6
	QD1	93	HEM	QT4	6.8
76 ALA					
	HN	76	ALA	HA	4.2
	HN	76	ALA	QB	3.8
	HN	77	LYS+	HN	5.6
	HN	81	ALA	QB	6.5
	HN	93	HEM	QT2	7
	HA	76	ALA	QB	3.4
	HA	77	LYS+	HN	3.2
	HA	77	LYS+	QD	7
	HA	80	GLU-	HB3	5
	QB	77	LYS+	HN	3.9
	QB	77	LYS+	HA	5.6
	QB	80	GLU-	HA	7
	QB	80	GLU-	HB2	6.3
	QB	80	GLU-	HB3	5.6
	QB	80	GLU-	HG3	7
	QB	81	ALA	HN	6.2
	QB	81	ALA	HA	5.6
	QB	93	HEM	QT2	5.1
77 LYS+					
	HN	77	LYS+	HA	3.4
	HN	77	LYS+	HB2	3.7
	HN	77	LYS+	HB3	3.7
	HN	77	LYS+	QG	7
	HN	77	LYS+	QD	7
	HN	80	GLU-	HN	4.3
	HN	80	GLU-	HB2	4.6
	HN	80	GLU-	HB3	4.4
	HN	81	ALA	HN	4.6
	HN	81	ALA	QB	4.6
	HA	77	LYS+	HB2	3.8
	HA	77	LYS+	HB3	3.8
	HA	77	LYS+	QG	6.6
	HA	77	LYS+	QD	6.9
	HA	81	ALA	HN	5.8
	HA	81	ALA	QB	4.1

	HB2	77	LYS+	QE	7
	HB2	78	GLY	HN	4.1
	HB3	77	LYS+	QG	6
	HB3	77	LYS+	QD	6
	HB3	81	ALA	HN	5.4
	HB3	81	ALA	QB	6.3
	QG	77	LYS+	QE	8
	QD	77	LYS+	QE	8
	78 GLY				
	HN	78	GLY	HA1	3.9
	HN	78	GLY	HA2	3.5
	HN	79	ALA	HN	5.6
	HN	80	GLU-	HN	6
	HN	81	ALA	HN	6
	HA1	80	GLU-	HN	5.5
	HA1	81	ALA	HN	5.7
	HA1	82	GLU-	HN	4.3
	HA2	79	ALA	HN	4.3
	HA2	80	GLU-	HN	5.6
	HA2	81	ALA	HN	6
	HA2	81	ALA	QB	4.6
	HA2	82	GLU-	HN	6
	79 ALA				
	HN	79	ALA	HA	4.5
	HN	79	ALA	QB	3.6
	HN	80	GLU-	HN	4.4
	HN	81	ALA	HN	6
	HA	79	ALA	QB	3.4
	HA	80	GLU-	HN	4.9
	HA	81	ALA	HN	6
	HA	82	GLU-	HN	4.3
	HA	82	GLU-	HB2	4.1
	HA	82	GLU-	HB3	3.8
	HA	82	GLU-	HG2	5.6
	HA	83	ALA	HN	4.7
	QB	80	GLU-	HN	4
	QB	80	GLU-	HA	5.3
	QB	81	ALA	HN	6.7
	80 GLU-				
	HN	80	GLU-	HA	4.1
	HN	80	GLU-	HB2	3.6
	HN	80	GLU-	HB3	4.3
	HN	80	GLU-	HG2	5.6
	HN	80	GLU-	HG3	4.8
	HN	81	ALA	HN	3.8
	HN	81	ALA	HA	6
	HN	81	ALA	QB	5.5
	HN	82	GLU-	HN	5.2
	HA	80	GLU-	HB2	4.5
	HA	80	GLU-	HB3	3.9
	HA	81	ALA	HN	4.9
	HA	82	GLU-	HN	4.7

	HA	83	ALA	HN	4.5
	HA	83	ALA	QB	4.1
	HA	84	VAL	HN	5.5
	HB2	81	ALA	HN	4
	HB3	80	GLU-	HG2	6
	HB3	81	ALA	HN	4.2
	HB3	81	ALA	HA	5.7
81 ALA					
	HN	81	ALA	HA	4.1
	HN	81	ALA	QB	3.4
	HN	81	ALA	HB3	4.3
	HN	82	GLU-	HN	3.9
	HN	82	GLU-	HB2	5.9
	HN	82	GLU-	HB3	6
	HN	82	GLU-	HG3	6
	HN	83	ALA	HN	4.6
	HA	81	ALA	QB	3.4
	HA	82	GLU-	HN	5.1
	HA	83	ALA	HN	5.7
	HA	84	VAL	HN	4.6
	HA	84	VAL	HB	4.1
	HA	84	VAL	QG1	7
	HA	84	VAL	QG2	7
	HA	85	ALA	HN	5.6
	QB	82	GLU-	HN	3.8
	QB	82	GLU-	HB2	7
	QB	82	GLU-	HG2	6.9
	QB	83	ALA	HN	6.2
82 GLU-					
	HN	82	GLU-	HA	4.4
	HN	82	GLU-	HB2	3.5
	HN	82	GLU-	HB3	3.7
	HN	82	GLU-	HG2	4.5
	HN	82	GLU-	HG3	5.9
	HN	83	ALA	HN	4.7
	HN	84	VAL	HN	4.4
	HA	82	GLU-	HB2	3.8
	HA	82	GLU-	HB3	3.9
	HA	82	GLU-	HG2	5.3
	HA	82	GLU-	HG3	5.3
	HA	83	ALA	HN	4.8
	HA	84	VAL	HN	6
	HA	85	ALA	HN	4.7
	HB2	83	ALA	HN	4.1
	HB3	83	ALA	HN	4.4
	HG2	83	ALA	HN	5.6
	HG2	85	ALA	QB	6.7
	HG3	83	ALA	HN	6
83 ALA					
	HN	83	ALA	HA	3.9
	HN	83	ALA	QB	3.4
	HN	84	VAL	HN	3.8

	HN	85	ALA	HN	5.7
	HA	83	ALA	QB	3.4
	HA	84	VAL	HN	4.8
	HA	85	ALA	HN	6
	HA	86	ALA	HN	4.4
	HA	86	ALA	QB	4.8
	HA	87	TRP	HN	5.3
	QB	84	VAL	HN	3.7
	QB	84	VAL	HA	5.6
84 VAL					
	HN	84	VAL	HA	4.2
	HN	84	VAL	HB	3.4
	HN	84	VAL	QG1	5.6
	HN	84	VAL	QG2	4.4
	HN	85	ALA	HN	3.8
	HN	85	ALA	HA	6
	HN	86	ALA	HN	5.7
	HA	84	VAL	HB	5
	HA	84	VAL	QG1	4.8
	HA	84	VAL	QG2	4.4
	HA	85	ALA	HN	5.3
	HA	86	ALA	HN	5.2
	HA	87	TRP	HN	4.5
	HA	87	TRP	HB3	4.2
	HA	87	TRP	HE3	5.4
	HA	88	LEU	HN	5.3
	HB	84	VAL	QG1	3.8
	HB	84	VAL	QG2	4
	HB	85	ALA	HN	3.9
	HB	93	HEM	QM1	7
	QG1	85	ALA	HN	6.4
	QG1	85	ALA	HA	7
	QG1	87	TRP	HN	7
	QG1	88	LEU	HN	7
	QG1	88	LEU	HB2	6.6
	QG1	88	LEU	HG	5.2
	QG1	88	LEU	QD2	5.6
	QG1	93	HEM	HDM	6.1
	QG1	93	HEM	QM1	4.6
	QG1	93	HEM	QT2	5.3
	QG2	85	ALA	HN	7
	QG2	93	HEM	HDM	7
	QG2	93	HEM	QM1	5.8
	QG2	93	HEM	QT2	5.8
85 ALA					
	HN	85	ALA	HA	4.1
	HN	85	ALA	QB	3.4
	HN	86	ALA	HN	4.1
	HN	87	TRP	HN	5.9
	HA	85	ALA	QB	3.5
	HA	86	ALA	HN	5.5
	HA	87	TRP	HN	6

86 ALA	HA	88	LEU	HN	5
	HA	88	LEU	HB2	4.2
	HA	88	LEU	HB3	4.9
	HA	88	LEU	QD1	4.9
	HA	89	ALA	HN	5.1
	QB	86	ALA	HN	3.8
	HN	86	ALA	HA	4.3
	HN	86	ALA	QB	3.4
	HN	87	TRP	HN	3.5
	HN	88	LEU	HN	5.5
	HA	86	ALA	QB	3.6
	HA	87	TRP	HN	4.7
	HA	89	ALA	QB	4.1
	HA	90	GLU-	HN	6
	QB	87	TRP	HN	3.7
	QB	87	TRP	HB2	7
	QB	87	TRP	HB3	7
87 TRP	HN	87	TRP	HA	4.7
	HN	87	TRP	HB2	3.6
	HN	87	TRP	HB3	3.7
	HN	87	TRP	HD1	6
	HN	88	LEU	HN	3.9
	HN	88	LEU	QD2	7
	HN	89	ALA	HN	4.6
	HA	87	TRP	HB2	4.2
	HA	87	TRP	HB3	3.9
	HA	87	TRP	HD1	5.4
	HA	87	TRP	HE1	6
	HA	88	LEU	HN	5.6
	HA	89	ALA	HN	5.7
	HA	90	GLU-	HN	5.4
	HA	90	GLU-	HB2	6
	HA	90	GLU-	HB3	5.6
	HB2	87	TRP	HD1	5.2
	HB2	87	TRP	HE3	4.6
	HB2	87	TRP	HE1	6
	HB2	88	LEU	HN	4
	HB3	87	TRP	HD1	4.7
	HB3	87	TRP	HE1	6
	HB3	88	LEU	HN	4.6
	HB3	88	LEU	HG	6
	HB3	88	LEU	QD2	7
	HD1	87	TRP	HE1	4.1
	HD1	90	GLU-	HG2	6
	HE3	87	TRP	HZ3	4.3
	HE3	88	LEU	HN	4.7
	HE3	88	LEU	HA	5
	HE3	88	LEU	HB2	5.2
	HE3	88	LEU	HB3	5.7
	HE3	88	LEU	HG	4.1

	HE3	88	LEU	QD1	5.8
	HE3	88	LEU	QD2	6
	HE1	87	TRP	HH2	6
	HE1	91	LYS+	HG2	6
	HE1	91	LYS+	QE	7
	HZ3	87	TRP	HH2	4.3
	HZ3	88	LEU	HG	5.6
	HZ3	88	LEU	QD1	6
	HZ3	88	LEU	QD2	6.2
	HZ2	87	TRP	HH2	4.2
	HZ2	91	LYS+	HG2	5.3
	HH2	88	LEU	QD2	7
	HH2	91	LYS+	HG2	5.7
	HH2	91	LYS+	QE	7
88 LEU					
	HN	88	LEU	HA	4.3
	HN	88	LEU	HB2	3.8
	HN	88	LEU	HB3	4.3
	HN	88	LEU	HG	5.3
	HN	88	LEU	QD1	5.8
	HN	88	LEU	QD2	7
	HN	89	ALA	HN	4
	HN	90	GLU-	HN	5.7
	HA	88	LEU	HB2	4.3
	HA	88	LEU	HB3	4.1
	HA	88	LEU	HG	5.4
	HA	88	LEU	QD1	6.1
	HA	88	LEU	QD2	4.7
	HA	89	ALA	HN	5.7
	HA	90	GLU-	HN	4.9
	HA	91	LYS+	HN	4.6
	HA	91	LYS+	HG3	4.5
	HB2	88	LEU	HG	4.4
	HB2	88	LEU	QD1	4.2
	HB2	88	LEU	QD2	5
	HB2	89	ALA	HN	4.4
	HB3	88	LEU	HG	5.4
	HB3	89	ALA	HN	4.6
	QD1	91	LYS+	HB2	6.6
	QD1	91	LYS+	HB3	4.8
	QD1	91	LYS+	QD	8
	QD1	93	HEM	QM1	5.5
	QD2	93	HEM	QM8	7
	QD2	93	HEM	QM1	7
89 ALA					
	HN	89	ALA	HA	3.9
	HN	89	ALA	QB	3.4
	HN	90	GLU-	HN	4.2
	HN	90	GLU-	HB2	4.6
	HN	91	LYS+	HN	5.3
	HN	91	LYS+	HB2	4.2
	HA	89	ALA	QB	3.4

90 GLU-	HA	90	GLU-	HN	5.3
	HA	91	LYS+	HN	5.3
	QB	90	GLU-	HN	4.3
	QB	90	GLU-	HB2	7
	QB	92	LYS+	QE	8
	HN	90	GLU-	HA	4.2
	HN	90	GLU-	HB2	4.5
	HN	90	GLU-	HB3	3.7
	HN	90	GLU-	HG2	5.6
	HN	90	GLU-	HG3	5.6
	HN	91	LYS+	HN	3.7
	HN	91	LYS+	HA	6
	HN	91	LYS+	HB2	5.6
	HA	90	GLU-	HB2	3.7
	HA	90	GLU-	HB3	4.3
	HA	90	GLU-	HG2	6
	HA	90	GLU-	HG3	5.2
	HA	91	LYS+	HN	4.6
	HA	92	LYS+	HN	6
	HA	92	LYS+	QG	7
	HA	92	LYS+	QD	7
91 LYS+	HA	92	LYS+	QE	6.9
	HB2	90	GLU-	HG2	4.5
	HB2	91	LYS+	HN	5
	HB3	90	GLU-	HG2	4.9
	HG2	92	LYS+	QE	5.7
	HN	91	LYS+	HA	4.2
	HN	91	LYS+	HB2	3.8
	HN	91	LYS+	HB3	4.1
	HN	91	LYS+	HG2	6
	HN	91	LYS+	HG3	5
	HN	91	LYS+	QD	7
	HN	91	LYS+	QE	7
	HN	92	LYS+	HN	6
	HN	92	LYS+	QD	6.5
	HA	91	LYS+	HB2	5.1
	HA	91	LYS+	HB3	4.1
	HA	91	LYS+	QD	7
	HA	92	LYS+	HN	4.1
	HB2	92	LYS+	HN	5.4
	HB3	92	LYS+	HN	4.6
92 LYS+	HG3	91	LYS+	QE	6.8
	HG3	92	LYS+	HN	5.6
	QE	92	LYS+	HB3	5.3
	HN	92	LYS+	HA	3.5
	HN	92	LYS+	HB2	5.1
	HN	92	LYS+	HB3	4
	HN	92	LYS+	QG	7
	HN	92	LYS+	QD	6.8

	HN	92	LYS+	QE	7
	HA	92	LYS+	HB2	4.3
	HA	92	LYS+	HB3	4.5
	HA	92	LYS+	QG	6.6
	HA	92	LYS+	QD	6.3
	HA	92	LYS+	QE	7
	HB2	92	LYS+	QE	7
	HB3	92	LYS+	QE	6.7
	QG	92	LYS+	QD	6.4
	QG	92	LYS+	QE	8
	QD	92	LYS+	QE	8
93 HEM					
	HAP71	93	HEM	HAP72	4.1
	HAP71	93	HEM	HBP73	5.5
	HAP71	93	HEM	HBP74	5
	HAP71	93	HEM	HGM	4.3
	HAP72	93	HEM	HBP73	5.4
	HAP72	93	HEM	HBP74	4.4
	HAP72	93	HEM	HGM	5
	HAP72	93	HEM	HAP61	6
	HAP72	93	HEM	HAP62	5.8
	HBP73	93	HEM	HBP74	3.8
	HBP73	93	HEM	HGM	4.8
	HBP73	93	HEM	HAP61	6
	HBP74	93	HEM	HGM	5.6
	QM8	93	HEM	HDM	4.2
	QM8	93	HEM	QM1	5.5
	HDM	93	HEM	QM1	4
	HDM	93	HEM	QT2	7
	QM1	93	HEM	HT2A	7
	QM1	93	HEM	QT2	4.2
	HT2A	93	HEM	QT2	4.3
	HT2A	93	HEM	HAM	3.8
	HT2A	93	HEM	QM3	5.8
	QT2	93	HEM	HAM	5.4
	QT2	93	HEM	QM3	7
	HAM	93	HEM	QM3	4.3
	HAM	93	HEM	QT4	7
	QM3	93	HEM	HT4A	7
	QM3	93	HEM	QT4	4.8
	HT4A	93	HEM	QT4	4.2
	HT4A	93	HEM	HBM	3.7
	HT4A	93	HEM	QM5	5.5
	QT4	93	HEM	HBM	5.2
	HBM	93	HEM	QM5	4.3
	QM5	93	HEM	HGM	7
	QM5	93	HEM	HAP61	5.8
	QM5	93	HEM	HAP62	5.2
	QM5	93	HEM	HBP64	5.3
	HGM	93	HEM	HAP61	4.3
	HGM	93	HEM	HAP62	5
	HGM	93	HEM	HBP63	5.2

HGM	93	HEM	HBP64	6
HAP61	93	HEM	HAP62	4.5
HAP61	93	HEM	HBP63	5.3
HAP61	93	HEM	HBP64	5.5
HAP62	93	HEM	HBP63	5.6
HAP62	93	HEM	HBP64	5.1
HBP63	93	HEM	HBP64	3.8

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Table 3: Dihedral angle constraints used in solution structure calculations.

23 ASP-	PHI	-145	-75
24 ALA	PHI	-105	-35
25 GLU-	PHI	-105	-35
28 VAL	PHI	-105	-35
30 GLN	PHI	-145	-75
31 LYS+	PHI	-145	-75
32 CYSS	PHI	-145	-75
34 SER	PHI	-105	-35
35 CYSS	PHI	-145	-75
36 HIS	PHI	-145	-75
43 ALA	PHI	-145	-75
45 ALA	PHI	-145	-75
47 ALA	PHI	-105	-35
48 ILE	PHI	-145	-75
50 LYS+	PHI	-145	-75
54 ASN	PHI	-145	-75
55 TYR	PHI	-145	-75
56 SER	PHI	-145	-75
58 GLU-	PHI	-105	-35
61 LEU	PHI	-105	-35
62 ASP-	PHI	-105	-35
64 ILE	PHI	-105	-35
66 ASN	PHI	-145	-75
76 ALA	PHI	-145	-75
77 LYS+	PHI	-145	-75
82 GLU-	PHI	-105	-35
83 ALA	PHI	-105	-35
75 ILE	PHI	-105	-35
89 ALA	PHI	-105	-35
90 GLU-	PHI	-145	-75
92 LYS+	PHI	-145	-75
22 VAL	PSI	100	180
23 ASP-	PSI	100	180
24 ALA	PSI	-70	0
25 GLU-	PSI	-70	0
26 ALA	PSI	-70	0
27 VAL	PSI	-70	0
28 VAL	PSI	-70	0
29 GLN	PSI	-70	0
30 GLN	PSI	-70	0
31 LYS+	PSI	-70	0
32 CYSS	PSI	-70	0
33 ILE	PSI	-70	0
34 SER	PSI	-70	0
35 CYSS	PSI	-70	0
39 ASP-	PSI	-70	0
44 SER	PSI	-70	0
47 ALA	PSI	-70	0

48 ILE	PSI	-70	0
49 ASP-	PSI	-70	0
50 LYS+	PSI	-70	0
53 ALA	PSI	-70	0
54 ASN	PSI	-70	0
55 TYR	PSI	100	180
56 SER	PSI	100	180
57 GLU-	PSI	-70	0
58 GLU-	PSI	-70	0
59 GLU-	PSI	-70	0
60 ILE	PSI	-70	0
61 LEU	PSI	-70	0
62 ASP-	PSI	-70	0
63 ILE	PSI	-70	0
64 ILE	PSI	-70	0
65 LEU	PSI	-70	0
75 ILE	PSI	-70	0
76 ALA	PSI	100	180
79 ALA	PSI	-70	0
80 GLU-	PSI	-70	0
81 ALA	PSI	-70	0
82 GLU-	PSI	-70	0
83 ALA	PSI	-70	0
84 VAL	PSI	-70	0
85 ALA	PSI	-70	0
86 ALA	PSI	-70	0
87 TRP	PSI	-70	0
89 ALA	PSI	-70	0
90 GLU-	PSI	-70	0
91 LYS+	PSI	-70	0

Table 4: N^{15} relaxation data of reduced cytochrome *c* from *Bacillus pasteurii* (T=296 K at 500 MHz).

Residue Nr	S^2	t_e (/ps)	R_{ex} (/s ⁻¹)
23	0.774	1591.0	
24	0.842		
25	0.830		
26	0.887		
27	0.876		
28	0.924		
29	0.937		
30	0.883		
31	0.834		
32	0.866		
33	0.896		
34	1.00		1.448
35	0.776		0.719
36	0.898		
37	0.882		
38	1.000		
39	0.915		0.765
40	0.963		
41	1.000		
42	0.922		
43	0.831		
44	1.000		
45	0.834		
47	0.848		
48	0.892		
49	0.913		
50	0.895		
51	0.884		
52	0.890		
53	0.911		
54	0.808		
55	0.847		
56	0.917		
57	0.868		
58	0.913		
59	0.944		
60	0.921		
61	0.921		
62	0.885		
63	0.907		
64	0.913		
65	0.925		
66	0.870		
67	0.895	263.16	
68	0.868		
69	1.000		
70	0.837		1.128
71	0.858		
73	0.838		
74	0.864		
75	0.992		

76	0.930		
77	0.838		
78	0.870		
79	1.000		
80	0.892		
81	0.876		
82	0.872		
83	0.867		
84	0.906		
85	0.917		
86	0.918		
87	0.905		
88	0.900		
89	0.915		
90	0.845		
91	0.810		
92	0.782		
HE1 87	0.751		
HD1 36	0.876		

Table 5: . The ratio of the opening constants (K^{op}) determined in the two oxidation states is shown on a per residue basis.

Residue number	K^{op}_{ox}/K^{op}_{red}
25	54.9
26	0.061
27	2.16
28	128
29	0.024
30	2.13
31	3.06
32	11.8
36	17.3
37	33.3
42	237
48	19.4
49	0.036
50	10000
51	3.11
52	3.68
53	4.02
55	0.785
56	3.41
59	3.96
62	202
63	50.9
64	257
65	34.9
66	6.34
67	6.82
68	5.65
71	8.96
74	0.089
75	7.10
76	2.96
80	170
81	572
82	1.56
83	2.22
84	31.9
85	244
86	0.025
87	286
88	23
89	230

90	2.08
91	0.116
92	0.068

Figure 1: ^{15}N - ^1H HSQC spectrum of reduced recombinant cytochrome *c* from *Bacillus pasteurii* at pH 7.