Table 2. Chemical shifts from partial assignment of ^{1}H NMR spectrum of oxidized *Ht* Cyt c_{552} determined to perform the magnetic axes calculation.

Residue	HN	Hα	Hβ	Others
N3				
E4				
Q5				
L6	7.74	3.84	1.56	Hγ 0.73, Qδ 0.14
A7	7.39	3.42	0.87	
K8	7.95	4.21	1.92, 1.73	Qε 3.34
Q9	8.36	3.94	2.20, 2.02	Hγ 2.48, 2.32
K10	7.85	4.20	1.73, 1.54	Qε 2.67
G11	7.54	4.13, 3.91		
C12	8.01	3.12	2.38, 2.55	
M13	8.41	6.42	3.02, 2.67	Hγ 3.73, 3.09
A14	7.93	4.53	1.55	
C15	8.11	5.69	4.01	
H16	10.55	8.80	11.38, 8.41	Hε 12.26
D17	10.55	6.00	3.91, 3.26	
L18	9.24		2.26, 2.05	Hγ 1.72, Qδ 1.41, 1.35
K19	8.69		1.94, 1.85	Qγ 1.50, Qδ 1.62, Qε 2.09
A20	9.19		1.67	
K21	8.87	4.56	2.08, 2.01	Hγ 1.56, Hδ 1.78, Hε 2.97
K22	8.44	4.85		Hε 3.35, others 2.55, 2.14, 1.96, 1.75
V23	7.85	3.61	1.25	Qγ 0.68, –0.33
G24	8.45			
P25				
A26	9.64	6.02	1.59	
Y27	9.64	4.45	3.08, 2.93	Qδ 6.95, Qε 6.39
A28	9.16	4.08	1.61	
D29	7.14	4.68	2.93	
V30	7.82	3.75	2.13	Qγ 0.74, 0.43
A31	8.23	3.74	1.61	
K32	7.38	4.06	1.95	Qγ 1.50, Qδ 1.79, Qε 3.04

Residue	HN	Hα	Hβ	Others
K33	7.59			Qε 3.91, others 1.33, 1.26, 1.00, 0.73, 0.53
Y34	7.24	4.48	3.27, 2.32	Qδ 7.11, Qε 6.72
A35	7.31	4.06	1.45	
G36	8.69	3.92		
R37	7.74	4.48	2.09, 1.96	Hγ 1.73, 1.61, Hδ 3.27, 2.86, Hε 8.15, Hη 6.47
K38				
D39	8.69	4.90	3.05, 2.60	
A40	7.30	3.71	1.52	
V41	8.28	3.12	1.90	Qγ 0.79, 0.75
D42	7.62	4.19	2.58	
Y43	8.42	4.08	3.10, 3.02	Qδ 6.60, Qε 6.72
L44	8.53	3.24	1.57	Hγ 1.37, Qδ 0.21, 0.12
A45	8.58	3.45	1.21	
G46	7.71	4.64, 3.20		
K47	7.48	5.33	2.90, 2.01	Hγ 1.27, Hδ 2.42, 1.79, Hε 3.64, 3.48
I48	8.57	4.37	1.38	Hγ 0.26, –3.20, Qγ –0.34, Qδ –0.72
K49	7.71	3.81	2.27, 1.87	
K50	9.53	5.19	2.78, 2.67	Hγ 2.04, Hδ 2.13, Hε 3.33
G51	10.62	9.01, 7.07		
G52	10.39	5.71, 4.94		
S53	8.63	4.36	3.62, 3.55	
G54	7.61	4.25, 3.73		
V55	9.83	3.67	1.98	Qγ 1.04, 0.27
W56	9.56	4.22	3.15, 2.24	Hδ1 6.20, Hε1 10.81, Hζ2 7.06, Hζ3 7.17, Hε3 7.56, Hη2 6.88
G57	7.40	3.93, 3.72		
S58	8.34	4.36	3.78, 3.67	
V59	6.94	3.84	0.90	Qγ 0.44, –0.14
P60				
M61	9.42		1.36	Qε –17.2, Hγ –20.2, –12.8
P62		5.67		2.20, 1.80
P63		5.83		4.21, 3.24, 2.76, 2.55
Q64	9.20	5.06	2.66	Hε 8.81, 6.70
N65	8.96	5.00	2.93, 2.71	Hδ 7.65, 6.93

Residue	HN	Hα	Hβ	Others
V66	7.62		2.17	Qγ 0.55, 0.33
T67	9.03	4.46		Qγ 1.23
D68	8.91	4.26	2.62	
A69	8.33	3.98	1.31	
E70	7.81		2.28	
A71	8.63	3.33	1.43	
K72	7.68	3.55	1.68, 1.27	Hγ 1.06, Hδ 1.49, Hε 2.78
Q73	7.75	3.84		
L74	8.28	3.55		Hγ 1.27, Qδ 0.15, –0.05
A75	7.73	2.90	1.08	
Q76	8.03	3.59	2.03, 1.86	Hγ 2.37, 2.20
W77	7.71	4.13	3.06	Hδ1 7.12, Hε1 10.32, Hζ2 7.26, Hη2 6.64, Hζ3 5.61, Hε3 6.72
I78	7.95	2.17	0.95	Hγ 0.89, –0.40, Qγ –0.40, Qδ –1.21
L79	7.28	3.62		Hγ 1.41, Qδ 0.67, 0.56
S80	7.46	4.31	4.01, 3.80	
I81	7.07	3.67	1.67	Hγ 0.84, Qδ 0.03
K82	7.78	4.23	1.84, 1.66	Hγ 1.38, HE 3.00

Heme assignments

1-CH_3	18.16	β-*meso*	–0.42	7–Hα1	12.98
2–Hα	1.26	5-CH_3	22.89	7–Hα2	2.20
2-CH_3	0.54	6–Hα1	3.60	7–Hβ1	
α-*meso*	1.54	6–Hα2		7–Hβ2	–1.13
3-CH_3	22.29	6–Hβ1		8-CH_3	24.28
4–Hα	0.25	6–Hβ2		δ-*meso*	–1.17
4-CH_3	1.20	γ-*meso*	9.07		

The sample was in 120 mM sodium acetate-d_3 buffer (pH 5.0), 5-fold excess of ferricyanide, at 300 K. Resultant pseudocontact shifts used in the calculation are reported in Table 4.