Supplementary Material

Summary of the measured (R_1_O_2, R_1_N_2, and ΔR_1) and the computed (b and AAREA) parameters for the 300 spectrally resolved protein protons of RNase A. The identity of each protein proton of the relaxation rate measurements is listed in the first column (H measured), while the scalar coupled proton shown as a cross-peak in the COSY spectra and its assignment is listed in the second column (H coupled) and the third columns. The residue types are in the fourth column. The measured protein proton spin-lattice relaxation rate constants and the associated standard errors in the fit (in the parentheses) when equilibrated with 11 atm pressure of oxygen and nitrogen are listed in the fifth (R_1_O_2) and the sixth (R_1_N_2) columns respectively. The differences in the protein-proton relaxation rate constants, i.e., the oxygen-induced relaxation rate (ΔR_1), are summarized in the seventh column. The distance of closest approach (b) between each protein proton and a surface molecular oxygen and the accessibility areas (AAREA) of each proton, computed from a protein structural model (7RSA), are listed in the last two columns.

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
1:HA	HB1	{3.98,1.63}	LYS	2.06(0.11)	0.64(0.04)	1.42(0.11)	2.60	16.2
1:HB1	HA	{1.62,3.99}	LYS	3.39(0.12)	1.54(0.04)	1.84(0.13)	2.60	11.1
2:HA	HB1	{4.52,1.85}	GLU	1.75(0.2)	0.47(0.08)	1.28(0.21)	2.60	10.1
2:HB1	HA	{1.85,4.53}	GLU	2.27(0.2)	0.91(0.05)	1.36(0.21)	2.60	14.1
2:HB2	HB1	{1.64,1.9}	GLU	3.47(0.53)	0.79(0.07)	2.68(0.53)	2.60	6.2
3:HB	HG1	{4.77,1.1}	THR	2.18(0.11)	0.49(0.03)	1.69(0.11)	2.60	10.1
3:HG1	HB	{1.09,4.79}	THR	3.38(0.44)	0.79(0.04)	2.59(0.44)	2.60	5.3
4:HA	HB1	{4.14,1.2}	ALA	2.92(0.1)	0.86(0.04)	2.05(0.11)	2.60	2.7
4:HB1	HA	{1.18,4.14}	ALA	3.73(0.13)	1.67(0.07)	2.06(0.15)	2.60	20.5
5:HA	HB1	{4.26,1.13}	ALA	2.03(0.13)	0.8(0.05)	1.22(0.13)	3.09	0
5:HB1	HA	{1.12,4.26}	ALA	3.34(0.11)	1.31(0.07)	2.03(0.12)	2.60	5.5
6:HA	HB1	{4.15,1.3}	ALA	2.92(0.08)	0.73(0.04)	2.19(0.09)	2.60	3.9
6:HB1	HA	{1.3,4.15}	ALA	2.87(0.08)	1.25(0.04)	1.62(0.09)	3.11	0
7:HA	HB2	{3.96,1.53}	LYS	1.55(0.43)	0.72(0.35)	0.83(0.55)	4.18	0
7:HB1	HB2	{1.78,1.56}	LYS	2.01(0.24)	0.76(0.09)	1.25(0.26)	2.60	0.5
7:HB2	HB1	{1.55,1.79}	LYS	2.78(0.52)	1.01(0.1)	1.77(0.52)	2.72	0.5
8:HA	HB1	{4.48,3.32}	PHE	1.54(0.19)	0.24(0.07)	1.3(0.2)	2.60	2.2
8:HB1	HA	{3.32,4.49}	PHE	2.07(0.12)	0.36(0.06)	1.72(0.14)	2.83	0
8:HB2	HB1	{2.85,3.35}	PHE	2.12(0.4)	0.42(0.12)	1.7(0.42)	2.93	0
8:HD1	HE1	{7.31,7.13}	PHE	12.24(1.97)	0.44(0.05)	11.8(1.97)	2.61	0.1
8:HE1	HD1	{7.12,7.3}	PHE	4.98(0.55)	0.42(0.04)	4.56(0.55)	4.53	0
9:HA	HB1	{3.68,2.15}	GLU	4.4(1.39)	0.35(0.09)	4.05(1.4)	3.80	0
9:HB1	HA	{2.14,3.68}	GLU	4.11(0.52)	0.57(0.06)	3.53(0.52)	2.60	4.9
10:HA	HB1	{4.19,1.78}	ARG	1.43(0.16)	0.27(0.05)	1.17(0.17)	2.60	6.8
10:HB1	HA	{1.77,4.2}	ARG	1.51(0.1)	0.34(0.03)	1.17(0.11)	2.60	7.9
11:HA	HB1	{3.76,1.15}	GLN	1.01(0.16)	0.43(0.09)	0.59(0.18)	6.02	0
11:HB1	HA	{1.15,3.78}	GLN	1.1(0.12)	0.29(0.07)	0.82(0.14)	3.63	0
12:HA	HB2	{4.99,1.45}	HIS	0.78(0.11)	0.17(0.07)	0.6(0.13)	6.15	0
12:HB1	HB2	{2.4,1.46}	HIS	1.57(0.12)	0.19(0.05)	1.39(0.13)	5.42	0
12:HB2	HA	{1.45,5}	HIS	1.73(0.08)	0.22(0.07)	1.51(0.11)	5.85	0
13:HA	HB1	{5.57,2.6}	MET	1.96(0.18)	0.16(0.06)	1.8(0.19)	4.64	0
13:HB1	HA	{2.59,5.57}	MET	2.89(0.34)	0.34(0.06)	2.55(0.34)	2.60	1.8
13:HB2	HB1	{1.51,2.61}	MET	1.47(0.37)	0.58(0.15)	0.89(0.4)	2.60	3.2
14:HA	HB1	{5.04,1.9}	ASP	0.75(0.08)	0.1(0.03)	0.65(0.09)	2.60	1
14:HB1	HA	{1.9,5.05}	ASP	0.78(0.12)	0.09(0.05)	0.69(0.14)	4.43	0
15:HA	HB2	{4.36,3.75}	SER	3.21(0.52)	0.18(0.05)	3.03(0.52)	2.60	0.5
15:HB1	HA	{3.91,4.37}	SER	2.03(0.27)	0.52(0.05)	1.51(0.27)	2.60	16.2

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
15:HB2	HA	{3.74,4.37}	SER	2.4(0.24)	0.22(0.04)	2.18(0.24)	2.60	8.1
17:HA	HB	{4.56,4.11}	THR	1.73(0.34)	0.35(0.11)	1.38(0.36)	2.60	6.8
17:HB	HG1	{4.11,0.74}	THR	2.05(0.09)	0.51(0.05)	1.54(0.1)	2.60	5.4
17:HG1	HB	{0.73,4.12}	THR	2.75(0.11)	1.11(0.05)	1.64(0.12)	3.99	0
18:HA	HB1	{4.26,3.75}	SER	2.38(0.46)	0.35(0.09)	2.03(0.47)	2.60	4.2
18:HB1	HA	{3.78,4.28}	SER	2.35(0.24)	0.63(0.1)	1.72(0.26)	2.60	14.3
19:HA	HB1	{3.09,0.65}	ALA	1.62(0.13)	0.41(0.04)	1.21(0.14)	3.93	0.4
19:HB1	HA	{0.62,3.12}	ALA	3(0.21)	0.7(0.04)	2.29(0.21)	2.60	13.1
20:HA	HB1	{3.38,0.47}	ALA	1.87(0.09)	0.53(0.03)	1.34(0.09)	3.98	0
20:HB1	HA	{0.46,3.4}	ALA	4.53(0.27)	1.15(0.1)	3.38(0.29)	2.60	0.8
21:HA	HB1	{4.25,3.93}	SER	4.82(1.45)	0.42(0.08)	4.39(1.45)	2.60	11.1
21:HB1	HB2	{4,3.76}	SER	2.68(0.2)	0.31(0.04)	2.37(0.2)	2.60	14.6
21:HB2	HB1	{3.74,3.99}	SER	2.83(0.16)	0.3(0.03)	2.54(0.16)	2.60	15.5
22:HA	HB1	{4.79,4.09}	SER	29.57(>10)	0.61(0.09)	28.96(>10)	2.60	11.1
22:HB1	HB2	{4.09,3.86}	SER	3.1(0.15)	0.8(0.02)	2.3(0.16)	2.60	13.1
22:HB2	HB1	{3.87,4.12}	SER	3.7(0.26)	1.01(0.09)	2.69(0.27)	2.60	10.3
23:HA	HB1	{4.42,4.12}	SER	2.58(0.68)	0.34(0.08)	2.24(0.69)	2.60	4.5
23:HB1	HB2	{4.14,4}	SER	3.13(0.28)	0.66(0.05)	2.47(0.28)	2.60	10.1
23:HB2	HB1	{3.98,4.12}	SER	2.77(0.18)	0.76(0.03)	2.01(0.18)	2.60	18.8
24:HA	HB1	{5.04,2.77}	ASN	2.06(0.13)	0.37(0.06)	1.69(0.15)	2.97	0
24:HB1	HA	{2.75,5.04}	ASN	1.82(0.15)	0.72(0.07)	1.1(0.17)	2.60	0.8
24:HB2	HA	{2.51,5.06}	ASN	2.65(0.46)	0.78(0.13)	1.88(0.48)	2.60	0.6
25:HB1	HB2	{3.32,2.75}	TYR	2.82(0.47)	0.33(0.08)	2.49(0.48)	2.60	1
25:HA	HB2	{4,2.77}	TYR	3.87(0.47)	0.32(0.08)	3.56(0.48)	2.62	0.4
25:HB2	HA	{2.77,4.02}	TYR	1.87(0.18)	0.37(0.05)	1.49(0.19)	4.23	0
25:HD1	HE1	{7.46,6.74}	TYR	2.35(0.1)	0.42(0.04)	1.93(0.11)	2.60	7.5
25:HE1	HD1	{6.73,7.47}	TYR	1.26(0.07)	0.29(0.04)	0.97(0.08)	2.60	1.9
26:HA	HB1	{3.79,3.05}	CYS	0.83(0.13)	0.26(0.08)	0.57(0.15)	6.34	0
26:HB2	HB1	{1.89,3.06}	CYS	0.96(0.14)	0.19(0.08)	0.78(0.16)	6.06	0
26:HB1	HA	{3.05,3.79}	CYS	0.79(0.12)	0.17(0.06)	0.62(0.13)	5.25	0
27:HA	HB1	{4.43,2.67}	ASN	4.51(0.65)	0.18(0.05)	4.32(0.65)	2.71	0.4
27:HB1	HA	{2.7,4.45}	ASN	2.48(0.27)	0.23(0.07)	2.25(0.28)	2.73	0
28:HA	HB1	{4,1.75}	GLN	1.45(0.16)	0.32(0.06)	1.13(0.17)	2.60	9.3
28:HB1	HA	{1.77,4}	GLN	2.86(0.26)	0.75(0.03)	2.11(0.26)	2.62	0.3
29:HA	HB2	{4.12,0.53}	MET	0.97(0.13)	0.15(0.08)	0.82(0.15)	3.11	0
29:HB1	HB2	{1.03,0.57}	MET	2.55(0.33)	0.26(0.07)	2.29(0.34)	5.06	0
29:HB2	HA	{0.52,4.13}	MET	1.05(0.12)	0.04(0.07)	1.01(0.14)	5.15	0

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
30:HA	HB1	{4.27,1.41}	MET	1.09(0.15)	0.32(0.12)	0.77(0.19)	5.15	0
30:HB1	HA	{1.41,4.27}	MET	1.36(0.15)	0.35(0.07)	1.01(0.17)	2.61	0.3
31:HA	HB2	{4.31,1.04}	LYS	2.26(0.22)	0.48(0.05)	1.79(0.22)	3.11	0
31:HB1	HB2	{1.64,1.13}	LYS	2.97(0.09)	1.63(0.06)	1.35(0.11)	2.60	5.4
31:HB2	HB1	{1.11,1.65}	LYS	3.06(0.07)	1.53(0.03)	1.53(0.08)	2.60	3
32:HA	HB1	{4.19,3.91}	SER	2.43(0.62)	0.46(0.1)	1.97(0.63)	2.60	12.7
32:HB1	HA	{3.92,4.18}	SER	2.41(0.37)	0.61(0.04)	1.8(0.38)	2.60	22.3
32:HB1	HB2	{3.98,3.85}	SER	2.87(0.16)	0.45(0.03)	2.41(0.16)	2.60	22.3
32:HB2	HB1	{3.85,3.98}	SER	2.35(0.12)	0.48(0.02)	1.87(0.12)	2.60	15
33:HA	HB1	{4.45,1.54}	ARG	1.67(0.38)	0.25(0.1)	1.42(0.39)	2.60	2.3
33:HB1	HA	{1.53,4.46}	ARG	0.97(0.15)	0.23(0.03)	0.74(0.15)	5.29	0
34:HA	HB1	{4.86,3.02}	ASN	1.4(0.24)	0.42(0.11)	0.98(0.27)	2.60	2.1
34:HB1	HB2	{3.01,2.78}	ASN	2.82(0.1)	0.69(0.01)	2.14(0.11)	2.60	12.7
34:HB2	HB1	{2.77,3.02}	ASN	3.09(0.08)	0.64(0.01)	2.46(0.08)	2.86	0
35:HB1	HG	{1.76,1.33}	LEU	1.16(0.13)	0.41(0.05)	0.75(0.14)	4.58	0
35:HD11	HG	{0.49,1.28}	LEU	1.02(0.14)	0.78(0.09)	0.24(0.17)	5.47	0
35:HD21	HG	{0.36,1.25}	LEU	1.28(0.11)	0.52(0.03)	0.76(0.11)	2.67	0.1
35:HG	HD11	{1.24,0.5}	LEU	1.14(0.09)	0.51(0.03)	0.64(0.1)	4.85	0
36:HB	HG1	{4.93,0.84}	THR	1.64(0.1)	0.53(0.03)	1.1(0.11)	3.34	0
36:HG1	HB	{0.83,4.9}	THR	2.96(0.26)	0.96(0.07)	2(0.27)	2.60	2.6
37:HA	HB1	{4.19,1.54}	LYS	1.55(0.18)	0.8(0.16)	0.75(0.24)	2.60	10.9
37:HB1	HA	{1.49,4.18}	LYS	2.2(0.14)	1.03(0.08)	1.17(0.16)	2.60	1.5
38:HA	HB1	{4.39,2.55}	ASP	2.04(0.13)	0.3(0.03)	1.74(0.13)	2.60	4
38:HB1	HB2	{2.58,2.38}	ASP	2.92(0.14)	0.45(0.02)	2.47(0.15)	2.60	5.6
38:HB2	HB1	{2.38,2.59}	ASP	2.68(0.17)	0.41(0.04)	2.27(0.18)	2.60	13.9
39:HA	HB1	{3.51,1.47}	ARG	1.41(0.57)	0.01(0.09)	1.39(0.58)	2.60	2.1
39:HB1	HA	{1.46,3.52}	ARG	2.24(0.51)	0.48(0.12)	1.75(0.53)	2.60	10.6
40:HA	HB2	{4.8,2.57}	CYS	0.94(0.12)	0.28(0.06)	0.66(0.14)	4.80	0
40:HB2	HA	{2.54,4.81}	CYS	1.09(0.14)	0.25(0.06)	0.84(0.15)	4.06	0
41:HA	HB1	{4.49,1.31}	LYS	0.97(0.18)	0.45(0.21)	0.52(0.28)	3.45	0
41:HB1	HA	{1.29,4.52}	LYS	1.61(0.3)	0.5(0.09)	1.1(0.31)	2.60	3.1
43:HA	HB	{5.46,1.89}	VAL	1.29(0.11)	0.54(0.04)	0.75(0.12)	4.59	0
43:HB	HG11	{1.88,0.61}	VAL	3.82(0.16)	0.9(0.02)	2.92(0.16)	2.60	11.7
43:HG11	HB	{0.6,1.89}	VAL	4.29(0.16)	1.59(0.06)	2.7(0.17)	3.61	0
45:HA	HB	{5.21,1.95}	THR	1.01(0.08)	0.3(0.04)	0.7(0.09)	4.57	0
45:HB	HA	{1.95,5.22}	THR	1.18(0.13)	0.44(0.04)	0.74(0.13)	2.83	0
45:HG1	HB	{0.29,1.97}	THR	2.39(0.21)	0.97(0.15)	1.42(0.26)	2.86	0.6

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
46:HA	HB1	{4.88,2.42}	PHE	0.83(0.3)	0.46(0.14)	0.37(0.33)	6.87	0
46:HB1	HA	{2.44,4.88}	PHE	0.46(0.14)	0.02(0.07)	0.44(0.16)	7.85	0
46:HD1	HE1	{7.04,7.2}	PHE	0.78(0.09)	0.18(0.05)	0.59(0.1)	6.20	0
46:HE1	HZ	{7.19,6.85}	PHE	0.78(0.09)	0.23(0.05)	0.54(0.1)	6.31	0
46:HZ	HE1	{6.85,7.2}	PHE	0.74(0.07)	0.28(0.05)	0.46(0.09)	7.26	0
47:HA	HB	{4.25,2.27}	VAL	1.23(0.17)	0.33(0.07)	0.9(0.18)	7.64	0
47:HB	HG21	{2.26,0.57}	VAL	1.68(0.08)	0.47(0.05)	1.21(0.09)	7.35	0
47:HG11	HB	{0.66,2.28}	VAL	1.88(0.32)	0.68(0.06)	1.2(0.32)	6.31	0
47:HG21	HB	{0.53,2.27}	VAL	1.58(0.2)	0.55(0.1)	1.04(0.22)	6.96	0
48:HA	HB2	{5.45,2.96}	HIS	1.47(0.14)	0.1(0.08)	1.37(0.16)	3.60	0
48:HB1	HB2	{3.36,2.97}	HIS	2.33(0.15)	0.19(0.06)	2.14(0.16)	3.70	0
48:HB2	HA	{2.96,5.46}	HIS	1.53(0.12)	0.27(0.06)	1.26(0.14)	3.25	0
49:HA	HB1	{4.9,1.12}	GLU	2.22(0.19)	0.32(0.04)	1.9(0.2)	2.60	5.2
50:HB1	HB2	{4.24,4.04}	SER	2.12(0.1)	0.36(0.03)	1.75(0.1)	2.60	16.3
50:HB2	HB1	{4.03,4.26}	SER	2.16(0.09)	0.37(0.03)	1.79(0.09)	2.60	22.6
51:HA	HB1	{4.07,1.51}	LEU	6.83(0.9)	0.58(0.07)	6.24(0.91)	4.32	0
51:HB1	HA	{1.5,4.09}	LEU	4.16(0.46)	0.69(0.05)	3.47(0.47)	2.60	4.1
51:HD11	HG	{0.59,1.2}	LEU	3.51(0.37)	0.98(0.08)	2.53(0.38)	3.13	0
51:HD21	HB1	{0.65,1.64}	LEU	0.96(0.21)	0.2(0.08)	0.77(0.22)	2.60	7.7
51:HG	HD11	{1.2,0.57}	LEU	5.68(0.52)	0.83(0.05)	4.84(0.53)	2.64	0
52:HA	HB1	{4.1,1.06}	ALA	3.2(0.12)	0.69(0.04)	2.5(0.12)	2.60	0.9
52:HB1	HA	{1.05,4.12}	ALA	3.51(0.14)	1.2(0.05)	2.3(0.15)	2.60	18.8
53:HA	HB1	{4.37,2.89}	ASP	2.41(0.21)	0.32(0.04)	2.09(0.21)	2.60	2.1
53:HB1	HA	{2.86,4.38}	ASP	1.99(0.12)	0.43(0.05)	1.57(0.13)	3.28	0
53:HB2	HB1	{2.34,2.87}	ASP	2.93(0.17)	0.51(0.04)	2.43(0.18)	2.60	4.1
54:HA	HB	{3.68,1.97}	VAL	1.85(0.29)	0.56(0.06)	1.29(0.3)	4.88	0
54:HB	HA	{1.94,3.68}	VAL	20.95(3.22)	0.61(0.04)	20.34(3.22)	4.42	0
55:HA	HB1	{3.55,2.02}	GLN	3.92(0.79)	0.49(0.07)	3.42(0.79)	4.03	0
55:HB1	HA	{2,3.56}	GLN	4.94(0.43)	0.57(0.07)	4.36(0.43)	2.60	1.4
56:HA	HB1	{4.01,1.15}	ALA	2.23(0.06)	0.51(0.04)	1.73(0.08)	2.60	9.4
56:HB1	HA	{1.14,4.02}	ALA	2.72(0.08)	0.83(0.02)	1.89(0.08)	2.60	7
57:HA	HB	{2.83,1.91}	VAL	1.05(0.12)	0.38(0.05)	0.67(0.13)	4.69	0
57:HG11	HA	{0.71,2.91}	VAL	2.16(0.51)	0.65(0.14)	1.51(0.53)	5.49	0
57:HB	HA	{1.9,2.85}	VAL	1.46(0.08)	0.68(0.05)	0.78(0.09)	6.03	0
58:HA	HB1	{3.43,2.39}	CYS	0.86(0.11)	0.24(0.09)	0.62(0.14)	4.67	0
58:HB1	HA	{2.37,3.44}	CYS	1.27(0.08)	0.28(0.07)	0.99(0.11)	2.60	3.2
59:HA	HB1	{4.57,3.96}	SER	1.6(0.22)	0.21(0.06)	1.39(0.23)	2.60	9.9

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
59:HB1	HA	{3.95,4.57}	SER	2.42(0.21)	0.31(0.03)	2.1(0.22)	2.60	18
61:HA	HB1	{4.36,1.89}	LYS	1.56(0.14)	0.42(0.04)	1.13(0.15)	2.60	4.1
61:HB1	HA	{1.89,4.36}	LYS	2.01(0.1)	0.51(0.02)	1.5(0.11)	2.77	0.1
62:HA	HB2	{4.36,2.38}	ASN	1.36(0.14)	0.21(0.04)	1.15(0.14)	4.31	0
62:HB1	HB2	{2.64,2.38}	ASN	2.55(0.1)	0.4(0.03)	2.15(0.11)	2.60	4.8
62:HB2	HB1	{2.38,2.64}	ASN	2.72(0.16)	0.35(0.04)	2.37(0.16)	2.60	13.3
63:HB	HG21	{1.82,-0.06}	VAL	3.09(0.11)	0.82(0.05)	2.27(0.12)	2.60	10.3
63:HG21	HB	{-0.07,1.82}	VAL	1.93(0.14)	0.94(0.05)	0.99(0.15)	4.27	0
64:HA	HB1	{4.29,0.89}	ALA	3.55(0.17)	0.58(0.04)	2.97(0.17)	2.90	0
64:HB1	HA	{0.87,4.31}	ALA	3.96(0.17)	1.01(0.04)	2.96(0.17)	2.60	17.2
65:HA	HB2	{4.58,2.28}	CYS	1.42(0.2)	0.45(0.04)	0.97(0.21)	2.92	0
65:HB2	HA	{2.28,4.57}	CYS	1.95(0.21)	0.52(0.03)	1.44(0.22)	2.60	1.8
66:HA	HB1	{3.88,1.62}	LYS	2.43(0.31)	0.63(0.11)	1.8(0.33)	2.60	12.1
66:HB1	HA	{1.62,3.91}	LYS	2.41(0.17)	0.88(0.05)	1.54(0.17)	2.60	5.8
66:HB2	HA	{1.47,3.91}	LYS	1.92(0.69)	1.26(0.27)	0.66(0.74)	2.60	11.2
67:HA	HB2	{4.54,2.55}	ASN	1(0.1)	0.25(0.1)	0.75(0.14)	2.60	13
67:HB1	HB2	{3.08,2.49}	ASN	2.49(0.1)	0.23(0.03)	2.27(0.11)	2.60	13.8
67:HB2	HA	{2.52,4.54}	ASN	1.16(0.12)	0.24(0.06)	0.92(0.14)	2.60	20.3
68:HA1	HA2	{4.28,3.44}	GLY	3.02(0.17)	0.21(0.04)	2.82(0.18)	2.60	11.6
68:HA2	HA1	{3.43,4.3}	GLY	2.71(0.12)	0.2(0.04)	2.51(0.12)	2.60	13.8
69:HA	HB2	{4.36,1.89}	GLN	1.68(0.17)	0.46(0.03)	1.23(0.18)	2.60	8.6
69:HB2	HA	{1.89,4.36}	GLN	2(0.1)	0.5(0.02)	1.5(0.1)	2.60	1.7
70:HB	HG1	{4.74,0.77}	THR	29.36(5.54)	0.51(0.04)	28.84(5.54)	2.60	7.6
70:HG1	HB	{0.75,4.75}	THR	8.22(2.92)	1.04(0.07)	7.18(2.92)	2.60	18.9
71:HA	HB2	{4.98,2.39}	ASN	65.34(>10)	0.01(0.25)	65.34(>10)	2.60	1.3
71:HB1	HB2	{3.52,2.53}	ASN	2.02(0.11)	0.18(0.05)	1.84(0.12)	2.77	0
71:HB2	HB1	{2.53,3.53}	ASN	2.16(0.08)	0.14(0.04)	2.02(0.09)	2.60	17.9
72:HB1	HB2	{2.61,2.23}	CYS	3.06(0.45)	0.63(0.05)	2.42(0.45)	4.99	0
72:HB2	HB1	{2.23,2.58}	CYS	5.37(0.73)	0.69(0.05)	4.68(0.73)	4.58	0
73:HA	HB2	{5.16,1.83}	TYR	0.91(0.21)	0.26(0.09)	0.65(0.23)	6.23	0
73:HB1	HB2	{2.66,1.85}	TYR	0.76(0.16)	0.31(0.08)	0.45(0.18)	6.58	0
73:HB2	HB1	{1.86,2.66}	TYR	1.04(0.11)	0.31(0.04)	0.73(0.11)	5.54	0
74:HA	HB1	{5.52,1.38}	GLN	0.92(0.23)	0.2(0.09)	0.73(0.24)	5.08	0
74:HB1	HA	{1.36,5.51}	GLN	1.06(0.27)	0.53(0.18)	0.53(0.32)	3.67	0
75:HA	HB1	{4.7,3.95}	SER	1.33(0.17)	0.53(0.05)	0.79(0.18)	3.92	0
75:HB1	HA	{3.93,4.71}	SER	1.01(0.08)	0.54(0.05)	0.47(0.1)	2.61	0.4
76:HD1	HE1	{7.53,7.2}	TYR	2.81(0.08)	0.24(0.04)	2.57(0.09)	2.60	8

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
76:HE1	HD1	{7.18,7.56}	TYR	2.16(0.06)	0.26(0.04)	1.89(0.07)	2.60	7.4
77:HA	HB2	{4.92,3.73}	SER	1.98(0.16)	0.33(0.05)	1.65(0.17)	2.60	3.9
77:HB1	HB2	{3.9,3.72}	SER	3.1(0.06)	0.74(0.01)	2.36(0.06)	2.60	16.2
77:HB2	HA	{3.72,4.92}	SER	2.64(0.22)	0.64(0.05)	2(0.23)	2.60	10.8
78:HA	HB	{3.51,3.32}	THR	2.71(0.26)	0.59(0.07)	2.12(0.27)	4.71	0
78:HB	HG1	{3.51,0.24}	THR	1.37(0.08)	0.54(0.03)	0.83(0.09)	3.53	0
78:HG1	HB	{0.23,3.52}	THR	2.51(0.11)	1.06(0.05)	1.45(0.12)	2.60	14.5
79:HA	HB1	{4.6,1.43}	MET	1.27(0.14)	0.28(0.07)	0.99(0.16)	2.60	0.1
79:HB1	HA	{1.41,4.6}	MET	1.04(0.13)	0.31(0.06)	0.73(0.15)	5.24	0
80:HA	HB1	{4.9,4.07}	SER	1.64(0.22)	0.25(0.06)	1.39(0.23)	3.31	0
80:HB1	HA	{4.06,4.91}	SER	1.75(0.11)	0.31(0.07)	1.44(0.13)	2.60	9.7
81:HA	HN	{5.62,9.78}	ILE	1.43(0.24)	0.3(0.06)	1.13(0.25)	5.37	0
81:HB	HG11	{1.44,0.47}	ILE	1.54(0.11)	0.49(0.04)	1.05(0.12)	5.36	0
81:HG11	HB	{0.46,1.44}	ILE	1.17(0.2)	0.4(0.08)	0.77(0.21)	4.70	0
82:HA	HB	{5.2,3.82}	THR	2.39(0.18)	0.36(0.05)	2.03(0.18)	5.24	0
82:HB	HG1	{3.81,0.97}	THR	1.05(0.1)	0.43(0.06)	0.62(0.12)	7.02	0
82:HG1	HB	{0.96,3.82}	THR	1.93(0.18)	0.78(0.08)	1.15(0.19)	4.72	0.2
83:HA	HB1	{5.13,2.35}	ASP	1.69(0.2)	0.3(0.05)	1.39(0.21)	4.56	0
83:HB1	HA	{2.32,5.14}	ASP	7.05(1.29)	0.53(0.06)	6.52(1.3)	2.60	5.1
84:HA	HB1	{6.1,2.8}	CYS	0.88(0.1)	0.22(0.05)	0.65(0.12)	3.57	0
84:HB1	HA	{2.8,6.1}	CYS	0.74(0.1)	0.29(0.08)	0.45(0.13)	5.98	0
85:HB1	HA	{1.72,5.56}	ARG	3.08(0.62)	0.73(0.16)	2.35(0.64)	2.60	2.7
85:HB2	HA	{1.51,5.56}	ARG	2.69(0.65)	0.56(0.16)	2.12(0.67)	2.60	5.7
87:HB	HG1	{4.5,0.72}	THR	2.04(0.11)	0.42(0.04)	1.62(0.12)	2.60	12
87:HG1	HB	{0.71,4.52}	THR	2.13(0.15)	0.63(0.02)	1.5(0.15)	2.60	5.6
89:HA	HB1	{4.49,3.8}	SER	2.05(0.22)	0.28(0.05)	1.77(0.22)	2.60	8.1
89:HB1	HA	{3.81,4.5}	SER	2.5(0.28)	0.54(0.1)	1.96(0.3)	2.60	8.7
89:HB2	HB1	{3.69,3.81}	SER	4.53(0.32)	0.73(0.05)	3.8(0.32)	2.60	13.8
90:HA	HB1	{4.06,3.79}	SER	1.16(0.27)	0.34(0.11)	0.83(0.29)	2.99	0
90:HB1	HA	{3.78,4.04}	SER	2.08(0.21)	0.46(0.11)	1.61(0.24)	3.99	0
91:HA	HB1	{4.43,1.44}	LYS	1.54(0.16)	0.67(0.07)	0.87(0.18)	2.60	6
91:HB1	HA	{1.43,4.44}	LYS	2.45(0.12)	1.09(0.04)	1.36(0.13)	2.60	5.6
92:HA	HB2	{3.72,2.6}	TYR	1.1(0.13)	0.09(0.05)	1.01(0.14)	4.38	0
92:HB1	HB2	{3.33,2.59}	TYR	1.6(0.18)	0.04(0.05)	1.56(0.19)	2.60	4.9
92:HB2	HA	{2.58,3.73}	TYR	1.38(0.12)	0.15(0.05)	1.23(0.13)	2.60	11.2
93:HA	HB1	{3.13,0.78}	PRO	1.31(0.28)	0.03(0.08)	1.28(0.29)	3.21	0
93:HB1	HA	{0.79,3.14}	PRO	1.77(0.31)	0.17(0.1)	1.6(0.32)	2.60	13.7

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
94:HA	HB1	{4.96,2.55}	ASN	2.39(0.15)	0.34(0.04)	2.05(0.15)	2.60	6.6
94:HB1	HA	{2.56,4.97}	ASN	2.37(0.16)	0.56(0.02)	1.81(0.16)	2.60	3.1
95:HA	HB1	{4.66,2.79}	CYS	8.15(2.56)	0.1(0.06)	8.05(2.56)	4.56	0
95:HB1	HA	{2.79,4.68}	CYS	1.99(0.17)	0.17(0.05)	1.83(0.17)	2.60	2.4
96:HA	HB1	{4.81,0.88}	ALA	5.13(0.72)	0.6(0.04)	4.53(0.72)	2.63	0
96:HB1	HA	{0.85,4.82}	ALA	3.76(0.28)	1.14(0.05)	2.63(0.29)	2.86	0
97:HA	HB2	{4.93,2.12}	TYR	0.92(0.11)	0.32(0.1)	0.6(0.14)	4.69	0
97:HB1	HB2	{2.71,2.09}	TYR	1.5(0.15)	0.4(0.05)	1.09(0.15)	5.07	0
97:HB2	HB1	{2.09,2.71}	TYR	1.9(0.11)	0.46(0.04)	1.44(0.12)	5.80	0
98:HA	HB1	{4.82,1.65}	LYS	2.84(0.52)	0.65(0.11)	2.19(0.53)	2.60	2.4
98:HB1	HA	{1.64,4.82}	LYS	4.93(1.39)	0.87(0.09)	4.06(1.39)	2.60	4.5
99:HA	HB	{5.27,4.21}	THR	1.3(0.12)	0.33(0.05)	0.97(0.13)	4.22	0
99:HB	HA	{4.21,5.28}	THR	2.69(0.17)	0.49(0.04)	2.2(0.18)	2.61	0.7
99:HG1	HB	{0.95,4.21}	THR	3.71(0.24)	0.75(0.02)	2.96(0.24)	3.58	0
100:HA	HB	{4.67,4.09}	THR	3.21(0.27)	0.44(0.06)	2.77(0.28)	2.60	3.5
100:HB	HG1	{4.08,0.89}	THR	4.81(0.29)	0.61(0.04)	4.2(0.3)	2.69	0.3
100:HG1	HB	{0.89,4.09}	THR	5(0.29)	0.91(0.02)	4.09(0.3)	2.60	7.9
101:HA	HB1	{5.06,1.7}	GLN	2.79(0.36)	0.34(0.07)	2.45(0.37)	3.83	0
101:HB1	HA	{1.69,5.06}	GLN	3.44(0.38)	0.38(0.07)	3.06(0.39)	2.60	7
102:HA	HB1	{4.69,0.98}	ALA	3.92(0.46)	0.46(0.04)	3.46(0.46)	2.60	10.9
102:HB1	HA	{0.97,4.69}	ALA	8.16(1.35)	0.78(0.03)	7.38(1.35)	2.60	6.5
103:HA	HB1	{5.93,2.35}	ASN	1.22(0.12)	0.43(0.1)	0.79(0.15)	4.40	0
103:HB1	HB2	{2.36,2.09}	ASN	2.58(0.09)	0.7(0.03)	1.88(0.1)	2.60	14.4
103:HB2	HB1	{2.1,2.39}	ASN	3.16(0.23)	0.66(0.07)	2.5(0.24)	2.63	0.5
105:HA	HB2	{4.47,3.05}	HIS	1.13(0.17)	0.32(0.06)	0.81(0.18)	5.48	0
105:HB1	HB2	{3.21,3.05}	HIS	2.53(0.09)	0.91(0.04)	1.62(0.1)	3.60	0
105:HB2	HA	{3.04,4.48}	HIS	1.25(0.14)	0.39(0.05)	0.86(0.15)	4.56	0
106:HB	HG11	{1.5,0.67}	ILE	1.02(0.1)	0.4(0.04)	0.63(0.11)	7.01	0
106:HG11	HG21	{0.7,1.01}	ILE	2.08(0.16)	0.81(0.05)	1.27(0.17)	5.74	0
106:HG21	HG11	{1.03,0.71}	ILE	1.79(0.12)	0.79(0.05)	1(0.13)	6.04	0
107:HA	HB	{5.45,1.13}	ILE	0.93(0.26)	0.29(0.12)	0.64(0.28)	6.13	0
107:HB	HG11	{1.1,0.15}	ILE	1.15(0.14)	0.46(0.04)	0.69(0.14)	3.70	0
107:HG11	HB	{0.14,1.11}	ILE	1.14(0.11)	0.55(0.08)	0.59(0.13)	4.15	0
108:HA	HB	{4.86,1.85}	VAL	1.36(0.09)	0.3(0.07)	1.06(0.12)	6.69	0
108:HB	HG21	{1.76,0.22}	VAL	1.27(0.11)	0.52(0.03)	0.75(0.12)	6.93	0
108:HG21	HB	{0.2,1.74}	VAL	1.19(0.15)	0.65(0.09)	0.54(0.17)	7.73	0
109:HA	HB1	{5.54,1.07}	ALA	0.94(0.09)	0.35(0.05)	0.59(0.11)	4.95	0

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
109:HB1	HA	{1.06,5.55}	ALA	1.51(0.12)	0.48(0.04)	1.03(0.13)	2.60	0.4
110:HA	HB1	{5.46,2.4}	CYS	0.93(0.16)	0.2(0.05)	0.74(0.16)	5.89	0
110:HB1	HA	{2.4,5.46}	CYS	0.8(0.11)	0.15(0.06)	0.66(0.12)	5.06	0
110:HB1	HB2	{2.4,0.7}	CYS	0.86(0.12)	0.22(0.05)	0.64(0.13)	5.06	0
110:HB2	HB1	{0.7,2.4}	CYS	0.86(0.12)	0.3(0.06)	0.55(0.14)	5.39	0
111:HA	HB2	{4.67,1.54}	GLU	1.83(0.5)	0.43(0.11)	1.4(0.51)	2.60	1.9
111:HB1	HA	{1.75,4.67}	GLU	1.39(0.13)	0.53(0.03)	0.87(0.13)	2.60	2
111:HB2	HA	{1.56,4.68}	GLU	2.92(0.51)	0.76(0.08)	2.16(0.52)	2.60	7.3
112:HA1	HA2	{4.53,3.7}	GLY	2.32(0.11)	0.28(0.04)	2.04(0.12)	2.60	18.9
112:HA2	HA1	{3.68,4.55}	GLY	2.29(0.11)	0.27(0.04)	2.02(0.12)	2.60	12.5
113:HA	HB1	{4.77,2.68}	ASN	4.74(0.82)	0.31(0.04)	4.43(0.82)	3.13	0
113:HB1	HA	{2.77,4.79}	ASN	2.42(0.14)	0.49(0.03)	1.93(0.14)	2.60	13.6
114:HA	HB1	{4.68,2.1}	PRO	2.2(0.26)	0.45(0.07)	1.75(0.27)	2.60	3.6
114:HB1	HA	{2.1,4.68}	PRO	2.4(0.22)	0.43(0.03)	1.98(0.23)	2.60	2.9
115:HA	HB1	{4.23,2.76}	TYR	1.6(0.23)	0.27(0.08)	1.33(0.24)	4.26	0
115:HB1	HA	{2.75,4.24}	TYR	1.75(0.16)	0.37(0.05)	1.38(0.17)	2.60	8
115:HB2	HB1	{2.6,2.82}	TYR	1.07(0.08)	0.34(0.03)	0.73(0.08)	2.60	9.5
115:HD1	HE1	{7.47,7.01}	TYR	1.92(0.08)	0.32(0.04)	1.6(0.09)	2.63	0.4
115:HE1	HD1	{7,7.49}	TYR	1.6(0.06)	0.26(0.04)	1.34(0.07)	2.60	9.2
116:HA	HN	{4.91,7.9}	VAL	2.58(0.22)	0.43(0.03)	2.16(0.22)	3.57	0
116:HB	HG11	{1.89,0.42}	VAL	3.38(0.21)	0.61(0.04)	2.77(0.21)	2.60	0.8
116:HG11	HB	{0.4,1.89}	VAL	2.53(0.21)	0.91(0.09)	1.62(0.22)	2.60	3.3
117:HB2	HG2	{0.65,-0.28}	PRO	4.63(0.81)	0.44(0.07)	4.19(0.81)	4.59	0
117:HG2	HB2	{-0.28,0.65}	PRO	5.83(0.98)	0.36(0.09)	5.47(0.99)	4.21	0
118:HB	HG21	{1.73,0.11}	VAL	2.47(0.14)	0.98(0.05)	1.49(0.15)	2.61	0.5
118:HG21	HB	{0.09,1.75}	VAL	2.45(0.15)	1.16(0.08)	1.29(0.17)	3.49	0
119:HA	HB1	{5.71,3.18}	HIS	1.18(0.27)	0.19(0.08)	0.99(0.29)	2.60	3.2
119:HB1	HA	{3.17,5.72}	HIS	1.5(0.29)	0.26(0.06)	1.24(0.3)	2.60	10.5
120:HA	HB1	{4.33,2.54}	PHE	1.54(0.11)	0.32(0.06)	1.22(0.12)	4.90	0
120:HB1	HB2	{2.52,1.16}	PHE	1.14(0.24)	0.24(0.07)	0.9(0.25)	3.88	0
120:HB2	HB1	{1.15,2.53}	PHE	1.59(0.33)	0.3(0.07)	1.29(0.34)	2.60	1.4
120:HD1	HE1	{6.93,7.32}	PHE	1.96(0.07)	0.32(0.05)	1.65(0.08)	2.60	7.3
120:HE1	HD1	{7.31,6.95}	PHE	1.44(0.07)	0.41(0.04)	1.03(0.08)	2.60	3.8
121:HA	HB1	{4.74,1.97}	ASP	1.96(0.29)	0.32(0.05)	1.64(0.3)	2.60	0.6
121:HB1	HA	{1.96,4.74}	ASP	1.38(0.12)	0.42(0.04)	0.96(0.12)	4.41	0
122:HA	HB1	{4.48,1}	ALA	1.63(0.06)	0.36(0.05)	1.26(0.08)	2.60	4.9
122:HB1	HA	{0.99,4.49}	ALA	1.61(0.05)	0.49(0.03)	1.12(0.06)	2.80	0

H measured	H coupled	assignment (ppm)	residue type	$R_{1\_}O_2$ (s^{-1})	$R_{1\_}N_2$ (s^{-1})	ΔR_1 (s^{-1})	b (Å)	AAREA ($Å^2$)
123:HA	HB1	{5.41,3.78}	SER	1.1(0.22)	0.23(0.19)	0.87(0.29)	4.62	0
123:HB1	HA	{3.78,5.42}	SER	1.38(0.44)	0.56(0.08)	0.82(0.44)	4.37	0
124:HA	HB	{4.29,1.74}	VAL	2.26(0.59)	0.62(0.18)	1.64(0.61)	2.60	6.2
124:HB	HA	{1.75,4.31}	VAL	2.31(0.29)	0.74(0.1)	1.57(0.3)	2.60	14