Supporting Information for:

Solid-state NMR Study of a 41 kDa Membrane Protein Complex DsbA/DsbB

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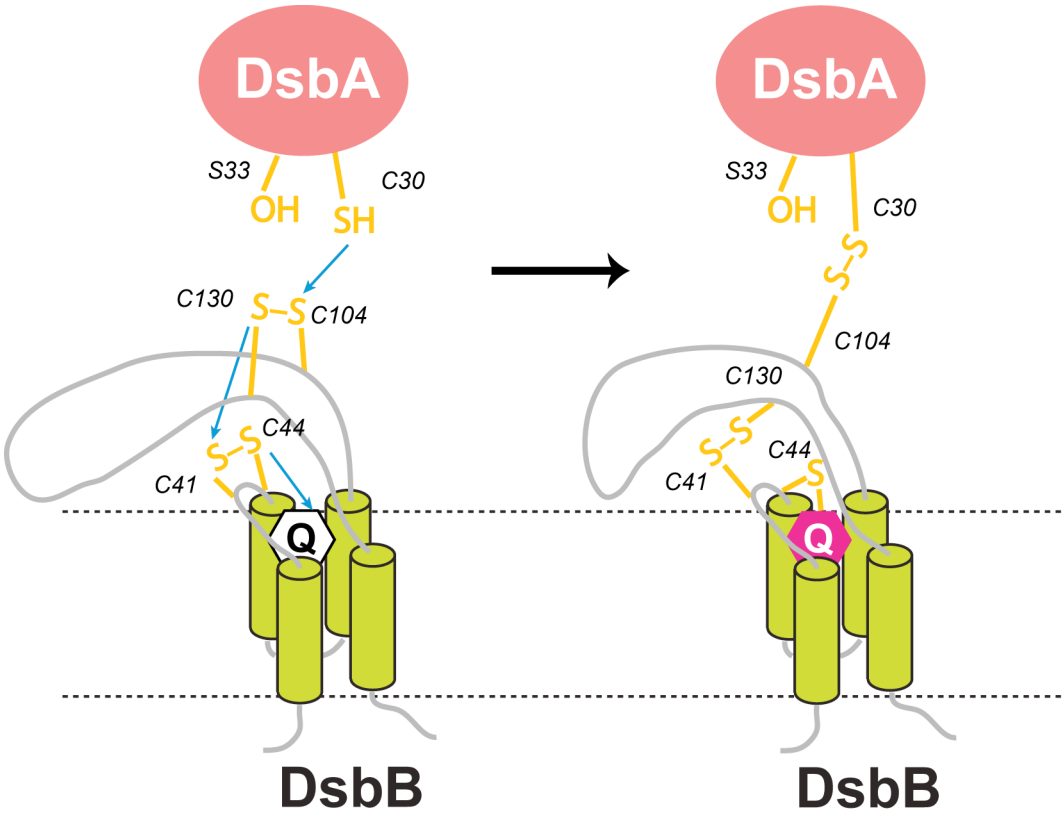

Figure S1. Schematic representation of the reaction of DsbA C33S mutant with wild-type DsbB to form a stable charge-transfer complex.

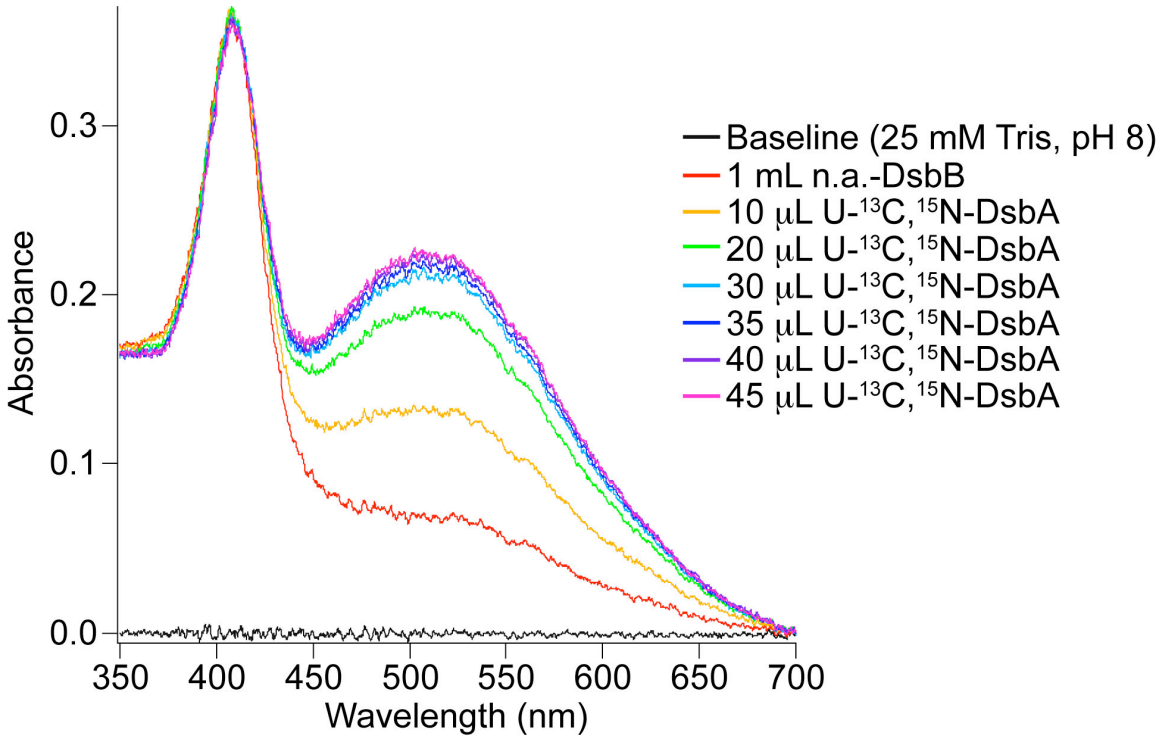

Figure S2. UV-Vis spectra acquired at varying points during titration of natural abundance-DsbB with U-^{13}C, ^{15}N-DsbA to complete 1:1 complex formation by monitoring peak formation at 500 nm.

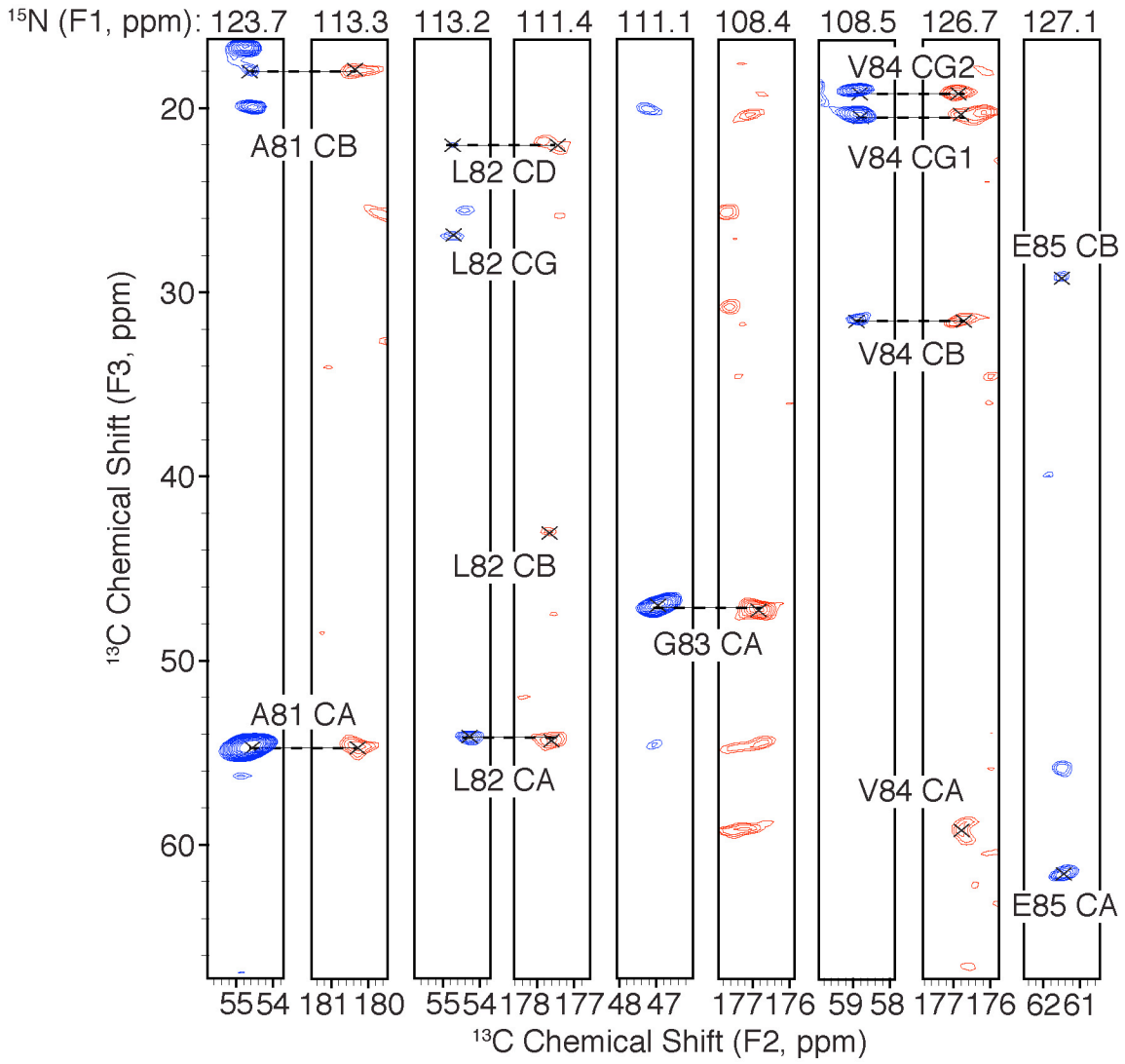

Figure S3. Backbone walk of DsbA(C33S) from Ala 81 to Glu 85 of U-^{13}C,^{15}N-DsbA(C33S) in complex with natural abundance wild type DsbB using NCACX (blue) and NCOCX (red) with 90 ms of DARR mixing acquired at 500 MHz (^{1}H frequency) at a MAS rate of 11.111 kHz at a sample temperature of -7 ± 1 °C. The spectra were processed with 50, 50, and 30 Hz and 40, 40, and 50 Hz Lorenzian-to-Gaussian apodization in F3, F2, and F1 for the NCACX (9 days) and NCOCX (13 days), respectively.

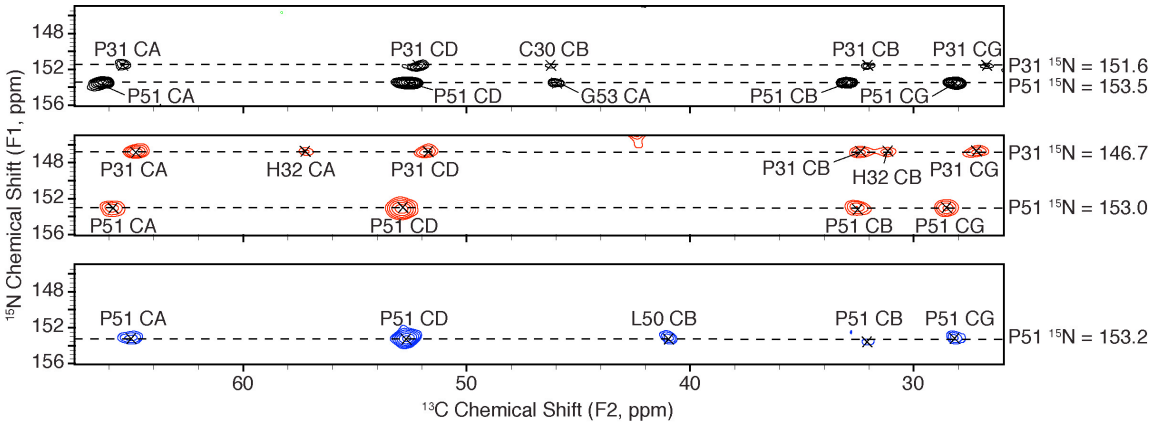

Figure S4. P31/P51 expansion of the ^{15}N-^{13}C 2D TEDOR followed by 90 ms DARR mixing spectra of oxidized wild type DsbA (black, 3.5 days), DsbA(C33S) (red, 4.5 days), and DsbA in complex with DsbB (blue, 3.75 days) with 1.80 ms TEDOR mixing acquired with a MAS rate of 13.333 kHz on a Infinity Plus 600 MHz (^{1}H frequency) spectrometer at a sample temperature of -6 ± 1 °C.

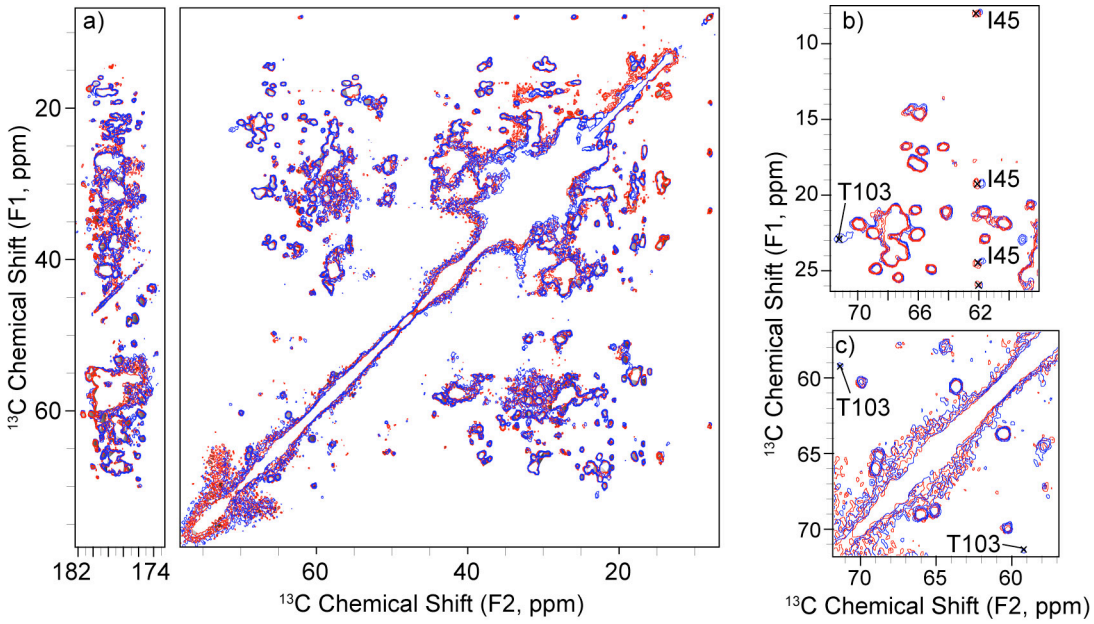

Figure S5. a) CC 2D with 25 ms DARR spectra acquired at MAS rates of 12.500 kHz at 750 MHz (^{1}H frequency) at sample temperatures of -12 ± 1 °C of U-^{13}C, ^{15}N-DsbB(C41S) (red, 1 day) and U-^{13}C,^{15}N-wild type DsbB in complex with natural abundance DsbA (blue, 5.25 days) and expansions of the b) methyl region, and c) Ser/Thr CA-CB regions with perturbed residues labeled.

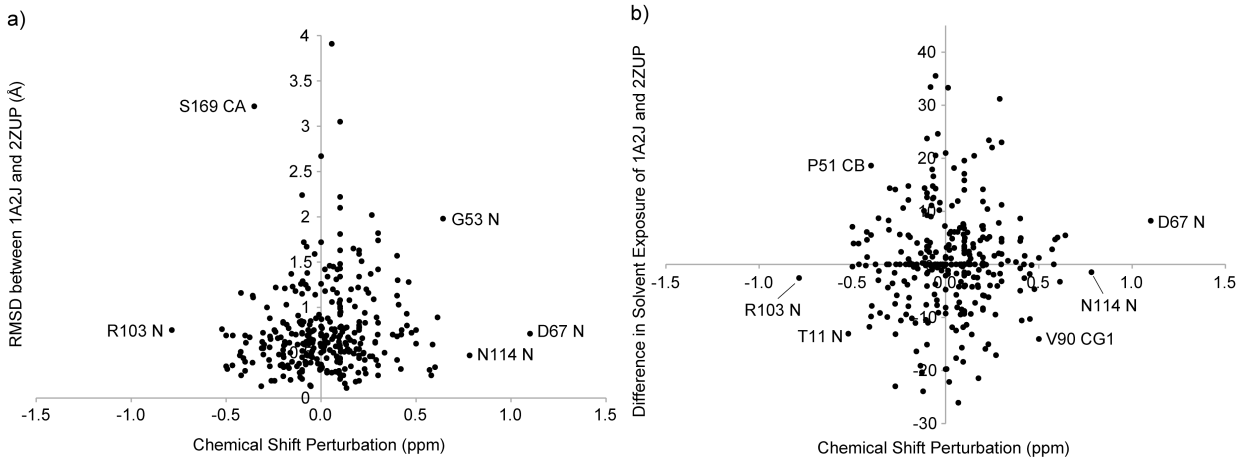

Figure S6. a) Individual atom RMSDs and b) difference in solvent exposure predicted from one of the modules of Shift X2 calculated based on the crystal structures of DsbA (PDB ID: 1A2J) and the DsbA/DsbB complex (PDB ID: 2ZUP) plotted against chemical shift perturbations of DsbA(C33S) versus DsbA(C33S)/DsbB complex.

Table S1. Chemical shift assignments (^{13}C and ^{15}N) for nanocrystalline, wild type oxidized DsbA, nanocrystalline, U-^{13}C,^{15}N-C33S mutant of DsbA, and membrane preparation U-^{13}C,^{15}N-DsbA in complex with DsbB. Differences in solvent exposure, predicted from one of the modules of Shift X2 and the RMSD differences between the crystal structures of DsbA (PDB ID: 1A2J) and the DsbA/DsbB complex (PDB ID: 2ZUP).

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
A1	C	176.3					-5.88	2.4
A1	CA	51.1	51.5		0.3		2.78	2.76
A1	CB	19.6	19.7		0.2		-5.67	5.33
A1	N	39.5					3.38	3.68
Q2	C	179.9	179.8		-0.2		6.18	1.68
Q2	CA	59.8	59.8		0.0		5.31	2.04
Q2	CB	29.9	29.9		0.0		7.89	2.76
Q2	CD	177.1					-28.97	5.06
Q2	CG	31.5	32.5		1.0		-12.28	4.62
Q2	N	121.6	121.2		-0.4		1.85	1.9
Y3	C	177.4	176.9		-0.5		-4.09	1
Y3	CA	58.5	57.9		-0.5		-0.04	1.48
Y3	CB	40.8	40.5		-0.3		-5.98	2.13
Y3	N	122.0	121.7		-0.3		-3.1	1.95
E4	C	174.4	174.6		0.2		-8.23	0.97
E4	CA	55.2	54.9	55.4	-0.3	0.5	-0.14	1.28
E4	CB	33.8	33.8		0.0		7.74	1.96
E4	CG	36.9		36.8				
E4	N	122.8	122.8		0.0		0.11	0.61
D5	C	177.3	177.4		0.0		-6.26	1.22
D5	CA	55.3	55.3		0.0		-6.73	0.99
D5	CB	41.2	41.4		0.2		-8.3	1.17
D5	CG	179.8	179.7		-0.1		-12.48	0.72
D5	N	125.8	125.6	125.8	-0.2	0.3	-4.08	1.09
G6	C	173.4	173.5	173.1	0.0	-0.4	-1.25	1.11
G6	CA	45.0	45.0	44.8	-0.1	-0.2	-16.41	1.37
G6	N	117.0	116.8	116.9	-0.2	0.1	-5.75	1.06
K7	C	175.6	175.5		-0.1		6.14	0.4
K7	CA	57.1	56.8	57.4	-0.3	0.6	4.69	0.59
K7	CB	32.1	32.2	32.0	0.0	-0.2	-6.29	0.58
K7	CG	25.4		25.1			9.82	0.38
K7	N	122.2	122.0	122.5	-0.1	0.5	-1.81	0.93
Q8	C	174.2	174.2	174.0	0.0	-0.2	0	0.45
Q8	CA	59.5	59.4	59.5	0.0	0.1	6.87	0.29
Q8	CB	27.2	27.2	27.0	-0.1	-0.2	4.02	0.4
Q8	CD	179.6					4.53	0.76
Q8	CG	34.2	34.1	33.6	-0.1	-0.5	-0.43	0.69

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
Q8	N	115.4	115.6		0.2		1.58	0.23
Y9	C	172.3	172.1	172.2	-0.1	0.1	-1.72	0.65
Y9	CA	55.2	55.1	54.8	-0.1	-0.3	-9.93	0.55
Y9	CB	41.3	41.6		0.3		-11.25	0.38
Y9	CD1	132.4	132.3		-0.1		-1.9	0.47
Y9	CD2	132.7					-9.3	0.76
Y9	CE	117.1	116.9		-0.2		-5.44	1.2
Y9	CG	128.3					0	0.37
Y9	CZ	158.0	158.1		0.1		-3.15	1.2
Y9	N	111.8	111.6	111.3	-0.2	-0.3	0	0.48
T10	C	174.5	174.5	174.5	0.0	0.0	-1.8	0.6
T10	CA	60.4	60.3	60.3	-0.1	0.0	-22.16	0.65
T10	CB	71.6	71.5	71.5	-0.1	0.0	-19.73	0.77
T10	CG2	22.2	22.1	22.0	-0.1	-0.1	9.25	2.24
T10	N	111.8	111.4	111.4	-0.3	0.0	-0.61	0.61
T11	C	175.4	175.3	175.4	-0.1	0.1	-18.38	0.67
T11	CA	62.9	62.8	62.9	0.0	0.1	-26.08	0.68
T11	CB	69.7	69.6	69.8	-0.1	0.2	-21.47	0.72
T11	CG2	21.7	21.8	21.7	0.1	-0.1	-15.13	0.81
T11	N	121.0	121.0	120.5	0.1	-0.5	-13.07	0.76
L12	C	177.5	177.4		-0.1		-15.49	0.55
L12	CA	55.9	55.8	56.1	-0.1	0.3	-17.12	0.46
L12	CB	41.6	41.6	41.5	0.0	-0.1	-20.35	0.35
L12	CD1	24.7	24.7	24.3	0.0	-0.4	-9.83	0.4
L12	CD2		23.6	23.5		-0.1	4.5	0.31
L12	CG	28.7	28.5	28.6	-0.2	0.1	-8.79	0.26
L12	N	129.3	129.2	129.3	-0.1	0.1	-15.71	0.44
E13	C	176.8	176.8		0.0		-11.47	0.76
E13	CA	58.6	58.7		0.2		-6.87	0.69
E13	CB	29.9	29.8		-0.1		20.2	1.01
E13	CG	32.5						
E13	N	123.4	123.1		-0.3		-11.44	0.65
K14	C	172.5	172.4		-0.1		-4.52	1.44
K14	CA	52.4	52.3		-0.1		-20.95	1.39
K14	CB	32.8	32.9		0.1		-4.14	1.55
K14	CG	24.5	24.4		-0.1		-15.57	1.6
K14	N	117.8	117.6	117.8	-0.1	0.2	-7.25	1.2
P15	C	176.5	176.4		-0.1		-2.56	1.15
P15	CA	62.6	62.3	62.5	-0.3	0.2	-15.94	1.51
P15	CB	32.7	32.7	32.6	0.0	-0.1	3.41	1.72
P15	CD	50.9	50.7	50.8	-0.2	0.1	-9.33	1.34
P15	CG	27.3	27.2	27.4	-0.1	0.2	0.27	1.59
P15	N	135.7	135.7	135.8	0.0	0.1	-8.5	1.42

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
V16	C	176.1	176.0	175.9	-0.1	-0.1	2.1	0.7
V16	CA	61.5	61.5	61.3	0.0	-0.2	-0.49	0.77
V16	CB	32.8	32.8	32.9	0.0	0.1	6.11	1.45
V16	CG1	21.6	21.6	21.7	0.0	0.1	3.33	3.05
V16	CG2	21.6	21.6	21.7	0.0	0.1	-1.84	0.4
V16	N	123.5	123.3	123.7	-0.2	0.4	-2.6	0.7
A17	C	179.0	178.9	179.0	-0.1	0.1	-4.22	0.76
A17	CA	52.6	52.4	52.2	-0.2	-0.2	5.62	0.75
A17	CB	18.9	18.9	19.2	0.1	0.3	-1.75	0.89
A17	N	132.4	132.4	132.8	0.0	0.4	0.43	0.7
G18	C	174.1	174.0		-0.1		-8.25	0.67
G18	CA	45.8	45.6	45.5	-0.2	-0.1	-23.93	0.91
G18	N	110.9	110.6	111.2	-0.4	0.6	-3.28	0.89
A19	C	175.2	175.1	175.3	-0.1	0.2	-3.94	0.49
A19	CA	50.5	50.3	50.4	-0.2	0.1	-3.29	0.46
A19	CB	17.3	17.3	17.3	0.0	0.0	-1.17	0.52
A19	N	122.3	122.4	122.1	0.1	-0.3	-7.44	0.56
P20	C	175.8					-0.21	0.42
P20	CA	62.5	62.4	62.6	-0.2	0.2	4.81	0.49
P20	CB	31.7	31.9	31.8	0.2	-0.1	12.57	0.6
P20	CD	50.3	50.1	50.3	-0.2	0.2	-0.24	0.77
P20	CG	27.8	27.8	27.9	0.0	0.1	19.55	0.55
P20	N	134.3	134.2	134.1	-0.1	-0.1	2.29	0.49
Q21	C	176.9	176.8		-0.1		0	0.27
Q21	CA	60.1	60.1		-0.1		-16.96	0.44
Q21	CB	29.8	29.6		-0.3		-14.34	0.6
Q21	CG	32.3	31.8		-0.5		-14.58	0.58
Q21	N	121.7	121.9		0.1		0.05	0.56
V22	C	173.0	173.0	172.9	0.0	-0.1	0	0.37
V22	CA	62.8	62.7	62.7	0.0	0.0	-6.76	0.45
V22	CB	34.0	33.6	34.1	-0.3	0.5	-4.68	0.72
V22	CG1	22.9	23.0	23.1	0.1	0.1	-8.89	1.48
V22	CG2	21.4	21.4	21.4	0.0	0.0	0	2.67
V22	N	116.1	116.0		-0.1		0	0.38
L23	C	173.4	173.4	173.4	0.0	0.0	0	0.74
L23	CA	52.8	52.8	52.5	0.0	-0.3	14.11	0.35
L23	CB	46.1	46.2	46.1	0.0	-0.1	14.28	0.13
L23	CD		22.4	22.5		0.1	-1.5	0.94
L23	CG	26.7	26.5	26.8	-0.2	0.3	1.94	0.36
L23	N	128.9	128.9	129.0	0.0	0.1	0	0.58
E24	CA	53.8					-0.29	0.49
E24	CB	34.0					0	0.43
E24	N	127.9					0	0.74

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
F25	C	175.7					0	0.28
F25	CA	56.3					0	0.21
F25	CG	139.9					0	0.46
F25	N	121.2					0	0.22
F26	C	170.7	170.2	170.4	-0.5	0.2	0	0.35
F26	CA	55.0	54.8	55.4	-0.2	0.6	5.06	0.34
F26	CB	43.7					0.98	0.25
F26	CD	131.3					0	0.54
F26	CE	130.8					0	0.66
F26	CG	136.4					0	0.33
F26	CZ	129.4					0	0.64
F26	N	119.8					0	0.45
S27	C	177.4	177.4	177.8	0.0	0.4	0	0.32
S27	CA	54.8	54.9	54.8	0.1	-0.1	0.25	0.59
S27	CB	64.6	65.4	65.3	0.8	-0.1	0	0.73
S27	N	108.9	108.2	107.8	-0.8	-0.4	0	0.67
F28	C	176.5					0	0.52
F28	CA	63.0					-5.55	0.53
F28	CB	38.5					0	0.57
F28	CD	132.2					0	0.59
F28	CG	139.3					0	0.53
F28	N	131.7	131.1	131.2	-0.6	0.1	0	0.57
F29	C	175.7					0	1.32
F29	CA	59.5					-2.23	1.19
F29	CB	39.8					-2.35	1.41
F29	CD	131.2					6.49	1.82
F29	CG	139.9					1.5	1.17
F29	N	115.9					0	1.28
C30	C	174.3					-0.03	0.89
C30	CA	52.7					-0.21	1.18
C30	CB	46.3					8.12	1.72
C30	N	120.4					0	1.18
P31	CA	66.3	66.3		0.0		19.33	0.67
P31	CB	32.1	32.3		0.2		25.79	0.88
P31	CD	52.0	51.6		-0.4		14.91	1.05
P31	CG	26.7	27.0		0.3		44.5	0.87
P31	N	151.5	146.7		-4.9		3.94	0.83
H32	C	177.8			-177.8		0	0.31
H32	CA	58.8	58.6		-0.2		17.77	0.4
H32	CB	29.6	29.7		0.1		22.96	0.42
H32	N	120.1	120.5		0.4		3.02	0.48
C33/S33	C	175.6					0	0.22
C33/S33	CA	63.3	63.5				-0.84	0.24

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
C33/S33	CB	33.7	65.1				-5.41	0.3
C33/S33	N	117.0					0	0.29
Y34	C	177.6					0	0.32
Y34	CA	58.8					6.28	0.22
Y34	CD	133.8					21.18	0.46
Y34	CG	127.7					1.63	0.25
Y34	N	123.8					0	0.16
Q35	C	179.0					2.36	0.44
Q35	CA	58.9					27.41	0.4
Q35	N	118.1					0	0.34
F36	C	176.4					0	0.31
F36	CA	60.2					23.09	0.27
F36	CB	38.6					11.7	0.24
F36	N	121.2					0.26	0.25
E37	C	177.8					0.61	0.56
E37	CA	58.6					17.67	0.54
E37	CB	30.9					10.68	1.1
E37	CG	34.7					3.29	1.8
E37	N	116.1					0	0.46
E38	C	176.7					8.73	0.79
E38	CA	58.8					16.9	0.89
E38	CB	30.8					13.21	1.01
E38	CG	34.9					13.3	0.6
E38	N	112.8					0	0.77
V39	C	176.9	176.9		0.0		16.05	0.56
V39	CA	64.0	64.0	64.0	0.0	0.0	33.29	0.55
V39	CB	32.7	32.3	32.6	-0.4	0.3	31.19	0.42
V39	CG1	20.9	20.9	21.1	0.0	0.2	11.84	0.44
V39	CG2	22.7					36.33	0.47
V39	N	116.6	116.6	116.5	0.0	-0.1	9	0.62
L40	C	176.3	177.0		0.7		5.68	1.22
L40	CA	55.2	55.2	55.4	-0.1	0.2	22.02	1.16
L40	CB	42.1	42.6		0.5		19.7	1.05
L40	CD	26.0	26.0		0.0		17.37	2.05
L40	CG	27.2	27.2	27.2	0.0	0.0	20.98	1.72
L40	N	115.0	114.9		-0.1		12.99	1.09
H41	C	176.7					1.68	1.1
H41	CA	55.8					6.2	1.23
H41	CB	25.6					22.08	1.6
H41	CG	131.1					20.4	1.14
H41	N	112.0					10.01	1.13
I42	CA	65.1					0.89	0.7
I42	CB	35.7					-1.11	0.62

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
I42	CD1	9.9					11.56	1.62
I42	CG1	27.1					2.21	0.92
I42	CG2	16.8					-7.88	0.71
I42	N	120.5					0	0.78
S43	C	176.5					3.13	0.57
S43	CA	57.5					18.3	0.49
S43	CB	61.4					6.96	0.41
S43	N	113.7					0	0.47
D44	C	177.9	178.4		0.5		7.31	0.63
D44	CA	57.5	57.4		-0.1		19.01	0.68
D44	CB	40.3	40.2		-0.1		27	0.81
D44	N	120.8	120.8		0.0		6.91	0.61
N45	C	178.3					2.75	0.41
N45	CA	56.9					0.01	0.54
N45	CB	40.1					-3.84	0.55
V46	C	178.1	177.9		-0.1		0	0.35
V46	CA	66.8	67.0	67.0	0.2	0.0	3.18	0.34
V46	CB	31.9	31.5	32.1	-0.4	0.6	2.83	0.31
V46	CG1	24.3	23.8	24.1	-0.5	0.3	11.21	0.25
V46	CG2	22.5	22.5	22.4	0.0	-0.1	3.34	0.29
V46	N	120.3	120.2		-0.1		0.78	0.33
K47	C	179.3	179.3		0.0		2.62	0.3
K47	CA	60.2	60.5		0.3		10.82	0.34
K47	CB	32.6	32.2		-0.5		13.18	0.45
K47	CG	25.3	25.1		-0.2		15.94	0.67
K47	N	119.8	120.5		0.6		4.13	0.37
K48	C	177.6	177.6		0.0		8.7	0.27
K48	CA	58.6	58.5		-0.2		5.87	0.26
K48	CB	33.0	33.0		-0.1		0.88	0.25
K48	CG		25.5					
K48	N	115.1	115.4		0.3		9.33	0.29
K49	C		176.2				0.14	0.45
K49	CA	55.7	55.5		-0.3		2.74	0.41
K49	CB		34.3				-3.9	0.22
K49	CG		25.9				-11.9	0.91
K49	N	116.8	116.5		-0.3		4.43	0.46
L50	C	174.4					5.96	0.34
L50	CA	53.0	53.3		0.3		-1.67	0.39
L50	CB	41.4	41.3	41.2	-0.1	-0.1	1.43	0.61
L50	CG	25.8	25.8		0.0		-1.59	0.42
L50	N	120.6	120.3		-0.3		4.82	0.42
P51	C	180.9					2.06	0.31
P51	CA	66.3	65.4	64.9	-0.9	-0.5	7.08	0.35

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
P51	CB	32.9	32.4	32.0	-0.5	-0.4	18.61	0.69
P51	CD	52.4	52.7	52.6	0.3	-0.1	13.43	0.45
P51	CG	28.1	28.4	28.1	0.3	-0.3	14.35	0.59
P51	N	153.5	153.0	153.2	-0.5	0.2	5.18	0.27
E52	C		180.0				10.17	1.19
E52	CA		59.3				9.19	0.45
E52	CB		28.0				12.69	1.53
E52	CG		34.4				16.52	2.24
E52	N		119.6				6.97	0.82
G53	C	174.1	174.1		0.0		4.29	2.82
G53	CA	45.5	45.7		0.2		18.05	3.37
G53	N	110.9	110.8	111.4	-0.2	0.6	5.46	1.98
V54	C	174.4	174.6		0.2		-3.62	1.27
V54	CA	62.5	62.5	62.5	-0.1	0.0	18.16	1.46
V54	CB	31.8	32.1	31.7	0.2	-0.4	8.7	1.13
V54	CG1	22.3	22.1	22.5	-0.2	0.4	-4.97	1.13
V54	CG2	21.7					3.12	1.67
V54	N	121.7	121.9		0.2	-121.9	1.72	2.17
M56	C	175.5					7.52	0.47
M56	CA	55.0					10.88	0.5
M56	CB	34.4					9.13	1.24
T57	C	171.9	171.8		-0.1		2.71	0.5
T57	CA	62.9	62.9	63.0	0.0	0.1	6.02	0.25
T57	CB	70.3	70.5	70.4	0.2	-0.1	14.37	0.28
T57	CG2	22.6	22.7	22.3	0.1	-0.4	5.53	0.3
T57	N	124.8	125.0		0.2		5.84	0.36
K58	CA	55.1					0	0.37
Y59	C	173.2					0	0.27
Y59	CA	52.1	52.1	52.1	0.0	0.0	0	0.28
Y59	CB	41.0		40.8			0	0.28
Y59	CD1	130.8					0	0.72
Y59	CD2	131.7					0	0.39
Y59	CG	129.9					0	0.29
Y59	N	124.5					0	0.29
H60	C	174.9					0	0.29
H60	CA	56.2					1.35	0.21
H60	CB	30.6					0	0.26
H60	CG	128.2					0	0.22
H60	N	123.5					0	0.18
V61	C	175.6	176.5		0.9		0	0.56
V61	CA	57.9	57.8		-0.1		-2.92	0.46
V61	CB	34.3	33.7		-0.6		6.96	0.53
V61	CG1	21.7					-3.37	0.38

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
V61	CG2	17.4					8.03	0.97
V61	N	111.5	110.6		-0.8		0	0.38
F63	CA	58.0					42.04	0.76
F63	N	111.1					9.82	0.66
M64	C	177.5					8.45	0.31
M64	CA	54.3					7.63	0.7
G65	C	175.5	176.6		1.1		9.11	0.77
G65	CA	47.5	47.5		0.1		21.99	0.57
G65	N	111.3					12	0.35
G66	C	176.9		177.1			10.81	0.94
G66	CA	45.6	45.6	45.5	0.0	-0.1	33.42	1.25
G66	N	109.2					15	0.76
D67	C	177.9	178.3		0.4		0.1	0.61
D67	CA	57.7	57.7		0.0		-2.81	0.58
D67	CB	39.9	39.8		-0.1		2.89	0.81
D67	CG	176.7					4.38	0.85
D67	N	128.2	128.0	129.1	-0.2	1.1	8.21	0.71
L68	C	179.2	179.0	179.2	-0.3	0.2	-0.06	0.66
L68	CA	57.0	57.2	57.1	0.2	-0.1	14.75	0.63
L68	CB	42.2	42.4		0.2		13.32	0.61
L68	CG	27.3	27.3		0.0		-0.47	0.65
L68	N	120.5	120.3		-0.1		3.05	0.62
G69	C	176.4	176.0		-0.4		0	0.69
G69	CA	48.2	48.1	48.0	-0.2	-0.1	17.89	0.69
G69	N	107.1	106.9	107.0	-0.3	0.1	2.08	0.44
K70	CA	59.8	59.8		0.0		8.17	0.37
K70	CB	31.8					-2.34	0.17
K70	CG		25.3				13.43	0.97
K70	N	121.5	121.2		-0.3		2.4	0.47
L72	C	178.1					0	0.45
L72	CA	57.7		58.0			0	0.41
L72	CB	42.7	42.5		-0.2		0	0.55
L72	CG	28.3	28.3	28.4	0.0	0.1	0	0.21
T73	C	176.6	176.5	176.8	-0.1	0.3	0	0.7
T73	CA	67.0	67.1	66.7	0.2	-0.4	6.1	0.51
T73	CB	68.6	68.5	68.5	-0.1	0.0	3.09	0.53
T73	CG1	22.1	22.4		0.3		3.6	0.82
T73	N	119.7	119.7		0.0		0	0.42
Q74	C	177.5	177.5		0.0		0	0.34
Q74	CA	59.6	59.5	59.7	-0.1	0.2	0	0.28
Q74	CB	26.0	26.0	25.9	0.0	-0.1	1.25	0.23
Q74	CD	177.5	177.3		-0.2		3.22	0.41
Q74	CG	31.0	31.0		0.0		-5.76	0.15

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
Q74	N	125.4	125.2	125.8	-0.1	0.6	0	0.25
Q74	NE2	108.4	108.0		-0.4		-4.99	0.49
A75	C	179.8	179.7		-0.1		0	0.48
A75	CA	54.9	54.9	54.7	0.0	-0.2	0	0.34
A75	CB	20.1	20.1	20.2	0.0	0.1	0.44	0.16
A75	N	123.4	123.3	123.4	-0.1	0.1	0	0.4
W76	C	177.8	177.9		0.2		0	0.21
W76	CA	59.1	59.3		0.2		0	0.47
W76	CB	29.7	29.4		-0.3		0	0.63
W76	CD1	128.0					0	0.68
W76	CD2	129.4					0	0.18
W76	CE1	140.0					0	0.19
W76	CE2	121.7					0	0.37
W76	CG	111.3					0	0.47
W76	N	120.6	120.7		0.1		0	0.54
W76	NE	128.8					0	0.52
A77	C	179.0	179.0		0.0		0	0.39
A77	CA	55.3	55.2	55.2	-0.1	0.0	-0.07	0.3
A77	CB	20.3	20.3	20.4	0.0	0.1	-0.42	0.28
A77	N	120.2	120.4	120.1	0.3	-0.3	0	0.13
V78	C	177.3	177.5	177.0	0.2	-0.5	0	0.69
V78	CA	67.3	67.2	66.9	-0.1	-0.3	-4.38	0.62
V78	CB	30.3	30.3	30.3	0.0	0.0	-0.28	0.75
V78	CG1	23.7	23.8	23.6	0.1	-0.2	-7.9	0.84
V78	CG2	22.3	22.3	22.3	0.0	0.0	-9.27	1.26
V78	N	119.8	119.7	119.7	-0.1	0.0	0	0.38
A79	C	179.8	179.9	179.8	0.1	-0.1	0	0.52
A79	CA	55.1	55.0	54.7	-0.1	-0.3	-5.84	0.19
A79	CB	17.8	17.8		0.0		-3.13	0.26
A79	N	121.1	121.0	120.8	0.0	-0.2	0	0.19
M80	C	179.4	179.4	179.4	0.0	0.0	-9.11	0.55
M80	CA	58.6	58.6	58.2	0.0	-0.4	-11.78	0.44
M80	CB	34.5	34.5	34.6	0.0	0.1	6.79	0.39
M80	CG	30.9	31.2	31.0	0.3	-0.2	12.13	0.48
M80	N	116.0	115.9	115.7	-0.1	-0.2	-0.16	0.2
A81	C	180.2	180.1	180.2	0.0	0.1	-11.85	0.62
A81	CA	54.8	54.7	54.6	-0.1	-0.1	-11.02	0.6
A81	CB	18.1	18.1		0.0		-15.96	0.59
A81	N	123.8	123.5	123.5	-0.2	0.0	-7.71	0.52
L82	C	177.5	177.5	177.6	0.0	0.1	-9.46	1.31
L82	CA	54.6	54.6	54.4	0.0	-0.2	-10.18	0.81
L82	CB	43.2	43.1	43.0	-0.1	-0.1	-10.46	1.26
L82	CD	22.0	22.0	22.1	0.0	0.1	3.45	2.22

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
L82	CG	27.0	26.8	27.0	-0.2	0.2	-5.83	1.63
L82	N	113.5	113.4	113.2	-0.1	-0.2	-9.44	0.67
G83	C	176.9	176.8	176.9	-0.1	0.1	-4.23	0.67
G83	CA	47.4	47.2	47.1	-0.2	-0.1	12.41	1.21
G83	N	111.4	110.9	111.3	-0.5	0.4	-10.58	1.03
V84	C	176.8	176.6	176.7	-0.2	0.1	-12.47	0.76
V84	CA	59.4	59.3	59.1	-0.1	-0.2	5.12	0.62
V84	CB	31.7	31.6	31.6	-0.1	0.0	5.78	1.18
V84	CG1	20.5	20.5	20.6	0.0	0.1	0.03	2.1
V84	CG2	19.2	19.2	19.3	0.0	0.1	2.62	0.92
V84	N	108.8	108.5	108.4	-0.4	-0.1	-5.67	0.81
E85	C	179.6	179.6	179.2	-0.1	-0.4	-3	0.39
E85	CA	62.0	61.7	61.5	-0.3	-0.2	-3.84	0.37
E85	CB	29.4	29.6	29.4	0.1	-0.2	-11.06	0.5
E85	CD	184.1	183.8		-0.3		-4.69	0.65
E85	CG	36.5	36.3	36.3	-0.2	0.0	-4.77	0.37
E85	N	126.7	126.3	126.8	-0.4	0.5	-10.3	0.8
D86	C	177.3	177.4	177.6	0.1	0.2	6.64	0.84
D86	CA	56.0	56.1	55.8	0.1	-0.3	6.51	0.55
D86	CB	39.8	39.7		-0.1		-7.47	0.25
D86	CG	179.9	180.1		0.2		8.21	0.9
D86	N	116.3	116.1		-0.2		1.92	0.71
K87	C	178.0	178.0	178.0	-0.1	0.0	1.13	0.44
K87	CA	57.3	57.3	57.4	0.0	0.1	3.84	0.51
K87	CB	34.3	34.1	34.4	-0.2	0.3	0.67	0.5
K87	CD	29.4	29.3	29.5	-0.1	0.2	5.11	1.34
K87	CE	39.8	39.9		0.1		-19.18	2.33
K87	CG	25.3	25.2	25.7	-0.1	0.5	1.22	0.75
K87	N	117.2	117.2		0.0		2.25	0.47
V88	C	176.1	176.1	175.9	0.0	-0.2	0	0.59
V88	CA	60.9	60.9	60.5	0.0	-0.4	-0.23	0.47
V88	CB	32.9	32.9	33.0	-0.1	0.1	-1.66	0.51
V88	CG1	19.5	19.3	19.5	-0.2	0.2	-8.58	0.19
V88	CG2	17.6	17.7	17.6	0.1	-0.1	-4.09	0.72
V88	N	104.0	103.7	103.5	-0.4	-0.2	0	0.36
T89	C	175.2	175.0		-0.1		0.15	0.42
T89	CA	69.3	69.4	69.1	0.1	-0.3	-1.6	0.42
T89	CB	69.8	69.8		0.0		-5.59	0.22
T89	CG2	21.3	21.4	21.4	0.1	0.0	1.43	0.32
T89	N	120.9	120.2		-0.7		0	0.52
V90	C	176.0	175.9	176.0	-0.1	0.1	4.97	0.51
V90	CA	69.4	69.2	69.4	-0.2	0.2	4.52	0.54
V90	CB	28.9	28.9	28.9	0.0	0.0	4.84	0.61

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
V90	CG1	24.4	24.2	24.7	-0.2	0.5	-14.07	0.6
V90	CG2	21.5	21.4	21.8	-0.1	0.4	8.64	0.68
V90	N	120.3	120.2		-0.1		3.11	0.52
P91	C	181.1					-0.06	0.43
P91	CA	65.9	65.6		-0.3		-0.06	0.51
P91	CB	31.6	31.6		0.0		2.45	0.48
P91	CD	49.1	49.1		0.0		19.58	0.81
P91	CG	27.8	27.8		0.0		2.71	0.54
P91	N	133.9	134.1	134.1	0.2	0.0	3.67	0.57
L92	C	177.9	177.9		0.0		0	0.49
L92	CA	58.1	57.9	58.0	-0.1	0.1	0	0.28
L92	CB	40.1	40.8	40.3	0.7	-0.5	3.93	0.32
L92	CD	22.9	23.1	23.1	0.2	0.0	0	0.69
L92	CG	27.0	27.0	27.1	0.0	0.1	0	0.43
L92	N	120.2	120.2		0.0		0	0.37
F93	C	180.1					0	0.43
F93	CA	64.0					8.99	0.43
F93	CB	39.5					8.17	0.26
F93	CD	132.1					0.39	0.37
F93	CG	141.6					0	0.24
F93	N	120.0					0	0.5
E94	C	180.4	180.3	180.2	-0.1	-0.1	10.09	0.38
E94	CA	59.4	59.5	59.4	0.0	-0.1	20.52	0.46
E94	CB	29.6	29.6		0.0		18.96	0.63
E94	CD		177.4				15.64	0.36
E94	CG	40.0					23.09	0.62
E94	N	116.2	116.0		-0.2		3.29	0.46
G95	C	175.8	175.8	175.5	-0.1	-0.3	0	0.65
G95	CA	46.7	46.4	46.2	-0.3	-0.2	10.61	0.66
G95	N	108.3	107.9	107.8	-0.4	-0.1	2.32	0.59
V96	C	178.2	177.9		-0.3		-0.46	0.71
V96	CA	66.5	66.5	66.5	0.0	0.0	6.11	0.84
V96	CB	32.2	32.0	32.2	-0.2	0.2	-1.04	1.01
V96	CG1	23.6	23.5	23.4	-0.1	-0.1	-1.74	1.15
V96	CG2	21.8	21.6		-0.2		-16.06	0.91
V96	N	119.7	119.8		0.1		0	0.93
Q97	CA		54.9				38.77	1.3
Q97	CD		172.0				1.8	0.9
Q97	NE2		111.2				0	0.94
K98	C	177.3					22.85	1.47
K98	CA	57.8					45.38	1.52
K98	CB	34.4					34.06	1.63
T99	C	175.6	175.7		0.1		5.4	1.55

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
T99	CA	62.2	62.2	62.1	0.0	-0.1	11.1	1.67
T99	CB	68.6	68.7	68.7	0.1	0.0	10.22	1.59
T99	CG2	22.2	22.3	22.4	0.1	0.1	4.35	1.81
T99	N	107.4	107.8		0.4		20.41	1.67
Q100	C	175.4	175.2	175.0	-0.2	-0.2	0.27	1.21
Q100	CA	57.3	57.5	57.4	0.2	-0.1	-1.54	1.29
Q100	CB	25.6	25.8	25.7	0.2	-0.1	-1.01	1.38
Q100	CD		180.7		180.7		1.94	0.96
Q100	CG	34.4	34.3	34.6	-0.1	0.3	4.84	1.42
Q100	N	114.7	114.6		-0.2		6.46	1.39
T101	C	175.3	175.5	175.4	0.2	-0.1	-0.21	0.82
T101	CA	60.9	60.9	60.5	0.0	-0.4	4.62	1.16
T101	CB	68.8	68.6	68.9	-0.1	0.3	1.61	1.37
T101	CG2	22.9	22.7	23.0	-0.2	0.3	-3.19	1.74
T101	N	106.1	105.8	105.6	-0.3	-0.2	-0.81	1.23
I102	C	174.0	174.0		0.0		0.47	0.93
I102	CA	60.8	60.8	60.7	-0.1	-0.1	-3.74	0.85
I102	CB	37.0	37.0	37.0	0.0	0.0	0	0.88
I102	CD1	14.8	14.6	14.9	-0.2	0.3	4.25	0.83
I102	CG1	27.2	27.2	27.3	0.0	0.1	0	0.99
I102	CG2	17.5	17.5	17.5	0.0	0.0	0	0.71
I102	N	121.1	121.1		0.0		-0.84	1.08
R103	C	175.4	175.4		0.0		-10.84	0.81
R103	CA	55.3	55.1	55.0	-0.1	-0.1	-19.11	1.18
R103	CB	32.7	32.4		-0.3		-18.26	1.88
R103	CD	40.9					32.97	2.68
R103	CG	27.2	27.0		-0.2		-2.53	2.37
R103	N	126.0	125.9	125.1	-0.1	-0.8	-2.57	0.75
S104	C	174.5	174.5		-0.1		-2.14	0.68
S104	CA	56.8	56.8	56.5	0.0	-0.3	-22.99	0.88
S104	CB	67.3	67.1	67.4	-0.1	0.3	-9.47	2.02
S104	N	115.1	114.9	115.0	-0.2	0.1	-9.35	0.78
A105	C	180.8	180.9	181.0	0.0	0.1	1.8	0.61
A105	CA	55.3	55.2	55.0	-0.1	-0.2	-10.59	0.73
A105	CB	16.9	17.1	17.1	0.1	0.0	-11.86	0.88
A105	N	123.7	123.6	123.5	-0.2	-0.1	-0.46	0.75
S106	C	176.3	176.3		-0.1		-5.33	0.52
S106	CA	61.5	61.4	61.3	-0.2	-0.1	16.59	0.69
S106	CB	62.3	62.3	62.5	0.0	0.2	23.39	0.83
S106	N	116.1	115.7	116.0	-0.4	0.3	2.07	0.62
D107	C	179.1	179.1	178.9	-0.1	-0.2	-0.29	0.33
D107	CA	57.0	57.1		0.1		5.62	0.3
D107	CB	42.5	42.6		0.1		-3.48	0.38

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
D107	N	120.3	120.3		0.0		-2.67	0.33
I108	C	177.0	177.0		0.0		0	0.17
I108	CA	65.8	65.8	65.6	0.0	-0.2	0.99	0.24
I108	CB	38.3	38.2	38.3	-0.1	0.1	7.62	0.3
I108	CD1	15.3	15.2	15.6	-0.1	0.4	-0.76	0.42
I108	CG1	29.0	29.0	28.9	0.0	-0.1	2.71	0.21
I108	CG2	18.4	18.7	18.5	0.3	-0.2	5.48	0.53
I108	N	120.1	120.0	120.0	-0.1	0.0	-0.31	0.32
R109	C	177.6					-0.86	0.38
R109	CA	59.2	59.4		0.2		-12.69	0.29
R109	CB	30.0					-12.38	0.3
R109	CD	43.2	43.3		0.1		5.27	0.65
R109	CZ	159.7					14.06	0.74
R109	N	121.1					0	0.34
D110	C	179.3	179.2		-0.1		-2.03	0.39
D110	CA	57.6	57.6		0.0		1.99	0.38
D110	CB	40.2	40.2		0.0		1.84	0.37
D110	CG	180.0					1.5	0.29
D110	N	116.5	117.2		0.7		-2.47	0.32
V111	C	179.3	179.1		-0.1		0	0.69
V111	CA	66.4	66.4	66.4	0.0	0.0	-1.17	0.43
V111	CB	30.9	30.9	30.7	0.0	-0.2	-2.53	0.61
V111	CG1	23.6	23.5	23.7	-0.1	0.2	1.29	0.8
V111	CG2	21.7	21.7	21.7	0.0	0.0	-2.13	0.57
V111	N	120.3	120.2		-0.1		-0.18	0.37
F112	C	177.8					0.97	0.43
F112	CA	62.1					4.55	0.37
F112	CB	38.1					0.01	0.34
F112	CG	142.3					0	0.32
F112	N	120.5					0	0.33
I113	C	182.3	182.2	182.4	0.0	0.2	-2.42	0.52
I113	CA	63.7	63.6	63.8	-0.1	0.2	-15.06	0.32
I113	CB	37.9	37.8	38.0	-0.2	0.2	-6.19	0.42
I113	CD1	13.7	13.5	13.8	-0.2	0.3	23	1.82
I113	CG1	28.3	28.3	28.3	0.0	0.0	-8.16	0.36
I113	CG2	17.1	17.3	17.4	0.2	0.1	-2.13	1.08
I113	N	122.1	122.1		0.0		-0.44	0.26
N114	C	176.3					4.21	0.98
N114	CA	55.6	55.6	55.7	0.0	0.1	-11.39	0.73
N114	CB	38.2	38.0	37.9	-0.2	-0.1	-7.62	0.85
N114	CG	176.7					4.29	3.06
N114	N	120.4	120.3	121.1	-0.1	0.8	-1.48	0.47
A115	C	177.0	176.9	176.9	-0.1	0.0	11.63	1.14

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
A115	CA	51.9	51.9	51.6	0.0	-0.3	-3.58	1
A115	CB	18.9	18.7	19.1	-0.2	0.4	4.95	1.3
A115	N	120.9	120.9	120.6	0.0	-0.3	8.27	0.72
G116	C	173.9	173.8	173.8	-0.1	0.0	2.7	1.42
G116	CA	45.3	45.1	44.9	-0.1	-0.2	2.35	1.22
G116	N	105.8	105.3	105.4	-0.4	0.1	7.46	1.05
I117	C	175.2	175.2		-0.1		5	1.01
I117	CA	61.0	60.8	61.0	-0.2	0.2	7.21	1.22
I117	CB	37.6	37.5	37.5	-0.2	0.0	11.05	1.34
I117	CD1	14.7	14.7		0.0		12.41	2.8
I117	CG1	25.8	25.8	25.9	0.0	0.1	17.07	1.63
I117	CG2	20.6	20.6	20.7	0.0	0.1	3.08	1.43
I117	N	125.4	125.4	125.5	0.0	0.1	3.17	1.08
K118	C	179.2	179.2	179.4	-0.1	0.2	-1.52	0.94
K118	CA	56.9	56.6		-0.2		-7.74	1.31
K118	CB	32.6	32.5		-0.1		-1.77	1.81
K118	CG	25.6	25.5		-0.1			
K118	N	125.8	126.1		0.3		6.91	1.24
G119	C	175.1	175.0		-0.1		-0.16	1.84
G119	CA	48.3	48.2		-0.1		6.36	1.71
G119	N	113.6	113.8	114.0	0.2	0.2	-2.51	1.65
E120	C	180.1					0.04	1.22
E120	CA	59.5	59.6		0.1		1.78	2.23
E120	CB	28.6	29.0		0.3		43.26	3.33
E120	N	117.3	117.3		0.0		6.73	1.61
E121	C	179.4					-3.39	0.6
E121	CA	58.3					-12.24	0.48
E121	CB	29.7					-5.24	0.33
E121	N	120.9					1.72	0.99
Y122	C	177.0					0	0.96
Y122	CA	62.9					-1.19	0.93
Y122	CB	38.0					-2.38	1.03
Y122	CE1	117.6					0	0.44
Y122	CE2	115.8					0.12	0.51
Y122	CG	127.1					0	0.69
Y122	N	122.7					-0.51	0.87
D123	C	178.7	179.9		1.2		-11.47	0.86
D123	CA	57.4	57.3		-0.1		-25.03	0.98
D123	CB	39.8	39.8		0.0		-8.3	1.12
D123	CG	180.1					6.66	1.45
D123	N	119.0	119.0		-0.1		0	0.97
A124	C	181.2	181.2		-0.1		-11.66	1.16
A124	CA	54.6	54.6		0.0		-15.79	1.19

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
A124	CB	18.1	18.2		0.0		-6.54	1.41
A124	N	121.0	121.0		0.0		-6.96	1.06
A125	C	181.1	181.1		0.0		0	0.64
A125	CA	55.1	55.0		-0.1		-7.32	0.65
A125	CB	18.5	18.5		0.0		1.56	0.99
A125	N	119.6	119.6		0.0		-3.99	0.68
W126	C	176.0	175.9		-0.1		3.84	0.65
W126	CA	61.5	61.1	61.5	-0.4	0.4	1.6	0.75
W126	CB	29.1		28.5			0.05	0.84
W126	CD1	127.7					12.86	1.07
W126	CD2	128.6					-0.15	0.64
W126	CE1	138.0					-1.86	0.68
W126	CE2	122.7					0.65	0.66
W126	CG	109.5					1.27	0.83
W126	N	121.9					0	0.81
W126	NE	130.9					8.98	0.97
N127	C	174.7	174.6		-0.1		3.61	0.53
N127	CA	53.4	53.2		-0.3		-3.53	0.65
N127	CB	40.3	40.2		-0.1		-12.73	0.58
N127	CG	177.5	177.6		0.1		0.09	0.83
N127	N	110.7	110.5		-0.2		-0.68	0.71
S128	C	175.5	175.6		0.1		3.78	0.57
S128	CA	59.3	59.1	58.7	-0.2	-0.4	-7.84	0.61
S128	CB	65.7	65.6	65.8	-0.1	0.2	-5.92	0.6
S128	N	116.5	116.1	116.2	-0.4	0.1	5.65	0.59
F129	C	178.8					4.52	0.29
F129	CA	61.7					-9.54	0.1
F129	CB	38.1					2.95	0.28
F129	CG	137.4					-6.45	2.38
F129	N	123.9					5.71	0.2
V130	C	177.2					-5.49	0.57
V130	CA	67.1	67.1	67.3	0.0	0.2	-4.29	0.62
V130	CB	31.6		30.4			-11.85	0.85
V130	N	119.9					-6.45	0.45
V131	C	177.5	177.7		0.2		0	0.27
V131	CA	67.2	67.0	67.2	-0.2	0.2	14.14	0.47
V131	CB	31.5	31.6	31.5	0.1	-0.1	12.63	0.83
V131	CG1	23.8	24.2		0.4		11.68	0.49
V131	CG2	22.4	22.9		0.5		5.19	1.3
V131	N	121.2	120.6		-0.6		-3.77	0.34
K132	C	180.3					3.32	0.49
K132	CA	59.9					22.79	0.31
K132	CB	32.0					5.46	0.24

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
K132	N	120.3					3.59	0.27
S133	C	176.7					0.34	0.45
S133	CA	61.2	61.2		0.0		0.12	0.3
S133	CB	62.1	62.4		0.3		-10.72	0.27
S133	N	115.2					-0.69	0.26
L134	C	181.4	181.4		0.0		0	0.58
L134	CA	57.6	57.6		-0.1		-1.13	0.55
L134	CB	44.2	44.0	44.1	-0.2	0.1	-13.22	0.54
L134	CD	22.7	22.9		0.2		-16.94	1.44
L134	CD1		26.2				-17.99	0.81
L134	CG	27.4	27.3	27.3	-0.1	0.0	-19.76	0.71
L134	N	124.0	123.8		-0.2		0	0.51
V135	C	177.1	177.1		-0.1		0.25	0.64
V135	CA	69.1	69.0	68.7	-0.1	-0.3	-13.16	0.68
V135	CB	31.5	31.4	31.5	-0.1	0.1	-3.98	0.79
V135	CG1	23.8	23.8	23.9	0.0	0.1	15.83	1.01
V135	CG2	21.1	21.0	21.4	-0.1	0.4	4.4	1.57
V135	N	123.3	123.2	123.0	-0.1	-0.2	0	0.71
A136	C	180.9	181.3		0.4		3.69	0.32
A136	CA	55.1	54.9		-0.2		6.27	0.43
A136	CB	17.8	17.8		0.0		0.09	0.58
A136	N	121.2	121.1	121.0	-0.1	-0.1	4.1	0.4
Q137	C	179.3	179.2		-0.1		0.41	0.44
Q137	CA	59.3	59.2		-0.1		3.56	0.31
Q137	CB	29.7	29.5		-0.2		-9.05	1.1
Q137	CG	33.8					3.66	1.13
Q137	N	118.7	118.5		-0.2		1.47	0.22
Q138	CA	59.9					3.27	0.14
Q138	N	119.4					0	0.23
E139	CA	59.8					11.87	0.33
E139	N	121.3					0.22	0.26
K140	C	177.7					4.05	0.32
K140	CA	59.0	58.8		-0.2		20.03	0.16
K140	CB	32.7	32.9		0.2		11.23	0.17
K140	CD		36.4				25.06	1.3
K140	CE		42.4				18.35	2.08
K140	CG	24.8	24.8		0.0		5.22	0.55
K140	N	122.3	122.2		0.0		1	0.39
A141	C	179.6	179.5	179.6	-0.1	0.1	0	0.59
A141	CA	55.0	54.8	55.1	-0.2	0.3	7.81	0.61
A141	CB	18.4	18.2		-0.2		6.75	0.72
A141	N	119.7					1.01	0.49
A142	C	178.9	178.8		-0.2		-0.56	0.36

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
A142	CA	54.4	54.5	54.0	0.0	-0.5	3.92	0.36
A142	CB	18.0	17.9		-0.1		8.95	0.39
A142	N	117.2	117.0	116.9	-0.2	-0.1	0	0.39
A143	C	182.5					3.69	0.49
A143	CA	54.6	54.3	54.4	-0.2	0.1	11.93	0.5
A143	CB	18.1	17.9		-0.1		7.83	0.63
A143	N	121.0	120.4		-0.6		1.57	0.44
D144	C	178.3	178.3	178.5	0.0	0.2	10.42	0.5
D144	CA	57.4	57.1		-0.3	-57.1	23	0.53
D144	CB	40.3	40.0		-0.2	-40.0	25.09	0.51
D144	CG	180.0					15.15	0.43
D144	N	120.9					4.21	0.55
V145	C	174.0	174.3		0.3		7.09	0.7
V145	CA	60.3	60.4	60.4	0.1	0.0	24.6	0.64
V145	CB	30.9	30.9	31.1	0.1	0.2	20.46	0.64
V145	CG1	20.3	20.2	20.1	-0.1	-0.1	23.72	0.71
V145	CG2	19.1	19.2	19.0	0.1	-0.2	14.76	0.83
V145	N	108.5	108.5	108.5	0.0	0.0	6.15	0.69
Q146	C	175.5					9.69	0.49
Q146	CA	56.0	56.0	55.9	0.0	-0.1	35.52	0.65
Q146	CB	26.2		26.2			44.31	0.71
Q146	N	118.2					5.79	0.63
L147	CA	56.4					19.22	0.39
L147	CB	43.1	43.0		0.0		13.43	0.36
L147	CG	26.9	27.0		0.1		7.59	0.39
L147	N	118.0					-0.56	0.5
R148	C	175.8	175.7		-0.1		17.61	0.38
R148	CA	55.0	54.6		-0.4		39.09	0.25
R148	CB	32.0	31.8		-0.1		48.51	0.7
R148	CG	27.0					55.98	1.4
R148	N	123.4					10.81	0.24
G149	C	171.1	170.8		-0.2		4.09	0.14
G149	CA	45.4	45.2		-0.2		53.17	0.31
G149	N	106.0	105.6		-0.4		5.73	0.33
V150	C	173.0	173.0		0.0		2.87	0.34
V150	CA	58.0	58.0	58.2	0.1	0.2	1.92	0.18
V150	CB	34.9	35.0		0.1		-0.31	0.3
V150	CG1	25.9		26.0			0	0.79
V150	CG2	19.0					4.65	0.26
V150	N	110.6	110.5		-0.1		1.42	0.23
P151	C	175.9					1.71	0.22
P151	CA	62.5					6.41	0.16
P151	CB	35.8					3.45	0.41

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
P151	CD	51.6					17.36	0.18
P151	CG						6.93	0.89
P151	N	133.8					4.36	0.25
A152	C	174.8	174.7		-0.1		0	0.12
A152	CA	51.9	51.8		-0.1		-5.27	0.31
A152	CB	25.6	25.4		-0.2		0.16	0.53
A152	N	122.8					0.14	0.16
M153	C	173.3	173.4		0.2		0	0.55
M153	CA	55.0					2.24	0.58
M153	CB	36.9	37.2		0.2		9.49	0.63
M153	CG	32.2	32.5		0.3		-4.8	0.48
M153	N	121.3	121.4		0.0		0	0.77
F154	C	176.4					0	0.45
F154	CA	56.0					0	0.35
F154	CB	43.9					0	0.29
F154	CD1	131.6					0	0.37
F154	CD2	130.1					0	0.29
F154	CG	139.7					0	0.19
F154	N	124.6					0	0.34
V155	C	176.0	176.1		0.1		0	0.18
V155	CA	60.8	60.8	60.9	-0.1	0.1	1.09	0.11
V155	CB	34.9	34.8	34.8	-0.1	0.0	0	0.31
V155	CG1	22.8	22.8	22.9	0.0	0.1	-4.18	0.78
V155	CG2	20.4	20.5	20.5	0.1	0.0	0	0.5
V155	N	123.0	123.0		0.0		0	0.17
N156	C	174.2	174.2	174.1	0.0	-0.1	-0.39	0.48
N156	CA	54.7	54.5	54.6	-0.2	0.1	-7.16	0.73
N156	CB	37.5	37.3	37.4	-0.2	0.1	-8.11	1.2
N156	CG	177.3	177.4		0.1		0.98	1.88
N156	N	127.1	127.2		0.1		0	0.48
G157	C	172.7	172.5	172.4	-0.2	-0.1	0	0.14
G157	CA	46.5	46.4	46.0	-0.1	-0.4	1.37	0.25
G157	N	105.7	105.2	105.3	-0.5	0.1	0	0.32
K158	C	175.0					0	0.48
K158	CA	57.2	57.1		-0.1		-24.34	0.38
K158	CB	37.6	37.3		-0.3		-23.78	0.81
K158	CG		29.9				-28.52	0.79
K158	N	114.7	114.5	114.3	-0.2	-0.2	0	0.36
Y159	C	174.7	174.9		0.2		0	0.59
Y159	CA	55.5					-8.59	0.57
Y159	CB	42.8					-2.11	0.57
Y159	CE	118.0					-11.07	0.67
Y159	CG	128.8					0	0.55

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
Y159	N	117.6					0	0.61
Q160	C	175.7	175.5	175.7	-0.2	0.2	-0.04	0.78
Q160	CA	53.4	53.4	53.4	0.0	0.0	-0.26	0.92
Q160	CB	30.7	30.7		0.0		5.28	0.83
Q160	CD	179.3	179.2		-0.1		3.11	0.99
Q160	CG	32.5	32.5		0.0		4.99	1.35
Q160	N		124.9				-0.79	0.92
Q160	NE2	108.8	108.3		-0.5		5.19	3.44
L161	C	177.7	177.4		-0.2		-0.24	0.69
L161	CA		54.1				0	1.01
L161	CB	40.5	40.8		0.3		0.13	1.07
L161	CD		24.2				0.79	1.17
L161	CG	28.3	27.9		-0.4		0	0.93
L161	N		131.3				0	1.14
N162	C	172.3	172.2		-0.1		0.35	0.61
N162	CA	49.9	50.0		0.2		3.23	0.25
N162	CB	38.6	38.6		0.0		3.46	0.33
N162	CG	177.5					-0.72	0.64
N162	N		118.5				0	0.52
P163	C	177.4					3.81	1.06
P163	CA	64.8	64.8	64.9	0.0	0.1	2.42	0.77
P163	CB	32.5	32.4	32.4	-0.1	0.0	7.22	0.6
P163	CD	50.8	50.8	51.0	0.0	0.2	7.25	0.54
P163	CG	27.8	27.9	28.0	0.1	0.1	14.03	0.69
P163	N	137.2	137.1		0.0		-0.56	0.37
Q164	C	177.2	177.1		-0.1		12.1	1.69
Q164	CA	58.1	57.6		-0.5		-0.45	1.44
Q164	CB	28.0	27.9		-0.1		-1.14	1.52
Q164	CD	173.9					34.44	2.89
Q164	N	114.9					5.23	1.28
G165	C	174.0	173.9		-0.1		6.22	1.28
G165	CA	44.7	44.7		0.0		7.57	1.34
G165	N	107.2	106.7		-0.5		10.58	1.16
M166	C	174.1					-6.61	1.06
M166	CA	54.5					-0.54	1.18
M166	CB	34.5					-2.14	0.85
M166	N	119.5	119.2		-0.3		-2.87	1.26
D167	CA	54.4					-12.72	1.81
D167	CB	40.5					-2.26	2.77
D167	CG	178.7					1	3.54
D167	N	121.1					-11.26	1.45
T168	C	175.5	175.6		0.2		-6.47	2.3
T168	CA	60.6	60.8		0.2		-14.24	1.71

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
T168	CB	68.8	68.6		-0.3		0.8	1.41
T168	CG2	22.5					-3.22	1.49
T168	N	112.4	112.3		-0.1		-11.65	1.53
S169	C	174.4					-3.35	2.63
S169	CA	61.1	61.4	61.0	0.3	-0.4	-9.17	3.22
S169	CB	63.3	63.3	63.4	0.0	0.1	-17.68	3.91
N170	CA	52.1					-22.91	0.76
M171	C	177.7					2.81	1.06
M171	CB	32.8					33.85	1.03
V173	CA	65.8	65.7	65.8	0.0	0.1	-0.25	1.16
V173	CB	32.2	32.1	32.3	-0.1	0.2	-3.98	1.2
V173	CG1		22.4				8.54	1.07
V173	CG2		21.3				-8.72	1.14
V173	N	121.6	121.4		-0.2		1.59	1.2
F174	C	176.2					0	0.72
F174	CA	61.8					-4.43	0.77
F174	CB		27.9				-4.3	0.63
F174	CG	138.9					0	0.7
F174	N	121.6					0	0.8
V175	C	177.6	177.7		0.1		0	0.75
V175	CA	67.0	66.9	66.8	0.0	-0.1	0.14	0.84
V175	CB	31.9	31.8	31.6	-0.1	-0.2	-0.01	1.03
V175	CG1	21.3	21.2	21.4	-0.1	0.2	-8.28	0.75
V175	CG2	24.4	24.1		-0.3		-2.79	1.28
V175	N	116.9	117.0	116.9	0.1	-0.1	0	0.84
Q176	C	178.4					-1.08	0.61
Q176	CA	58.8	59.0		0.2		-13.5	0.9
Q176	CB	28.2	27.7		-0.5		-17.03	1.15
Q176	CD	180.2	180.0		-0.2		-5.12	1.4
Q176	CG	34.4	34.2		-0.2		-18.86	1.48
Q176	N	116.7	116.5		-0.2		0.56	0.94
Q176	NE2	111.0	110.7		-0.3		-15.43	1.78
Q177	C	180.0	180.0		0.0		0	0.36
Q177	CA	59.3	59.0		-0.2		6.06	0.43
Q177	CB	28.2	28.0		-0.1		4.91	0.76
Q177	CG	34.4	34.2		-0.2		5.48	0.94
Q177	N	119.1					-1.06	0.6
Y178	C	177.9	178.1		0.2		0	0.39
Y178	CA	61.9	61.7		-0.2		-5.12	0.45
Y178	CB	38.3					-0.07	0.4
Y178	CE	117.4					0	0.49
Y178	CG	129.8					0	0.25
Y178	N	126.5	126.4		-0.1		0	0.45

Residue	Atom	Oxidized Wild Type	C33S	Complex	C33S vs. wt	Complex vs. C33S	Solvent Exposure	RMSD Difference
A179	C	179.7	179.7		0.0		0	0.48
A179	CA	55.5	55.3		-0.2		1.7	0.41
A179	CB	18.4	18.3		-0.1		6.78	0.52
A179	N	120.2					0	0.4
D180	C	179.7					0	0.63
D180	CA	57.4					7.4	0.47
D180	CB	40.0					7.42	0.42
D180	CG	179.5					-0.35	2.14
D180	N	118.7	118.8		0.1		-0.59	0.45
T181	C	176.4					0	0.29
T181	CA	67.5					0	0.28
T181	CB	67.6	67.5		-0.1		-1.43	0.33
T181	CG2	21.8	21.8		0.0		-3.21	0.32
T181	N	120.2					0	0.33
V182	C	177.6					0	0.86
V182	CA	67.7	67.8	67.8	0.1	0.0	0	0.87
V182	CB	30.7	30.8	30.9	0.1	0.1	0	0.95
V182	CG1	24.1	24.2	24.2	0.1	0.0	1.18	0.79
V182	CG2	22.5	22.9		0.4		0	1.04
V182	N	121.5	121.4		-0.2		0	0.82
K183	CA	60.5					8.29	0.9
K183	N	120.9					0	0.9
Y184	C	177.8	177.9		0.1		0	0.48
Y184	CA	60.5	59.9		-0.6		-8.44	0.49
Y184	CG	129.9					-3.08	0.25
Y184	N	120.1					0.28	0.56
L185	C	179.3	178.5		-0.8		0	0.5
L185	CA	56.6	56.4	56.7	-0.1	0.3	-1.94	0.46
L185	CB	42.2	42.4	42.2	0.2	-0.2	-3.16	0.48
L185	CD		23.5				-4.63	0.63
L185	CG	25.7	25.7	25.8	0.0	0.1	0	0.44
L185	N	118.1	118.1		0.1		0	0.44
S186	C	175.7					-2.36	0.83
S186	CA	61.9	62.0		0.1		-0.38	0.44
S186	CB	62.6	62.5		-0.1		-3.41	0.6
S186	N	115.0	115.0		0.1		0	0.51
E187	C	175.9					-9.86	0.44
E187	CA	56.1	56.0		-0.1		-3.78	0.94
E187	CB	30.1	30.4		0.3		13.57	1.48
E187	CG	36.8	36.7		-0.1		-7.18	2.08
E187	N	119.4	119.4		0.1		-4.14	0.76
K188	CA		57.6				20.12	0.69