

Supplementary Material

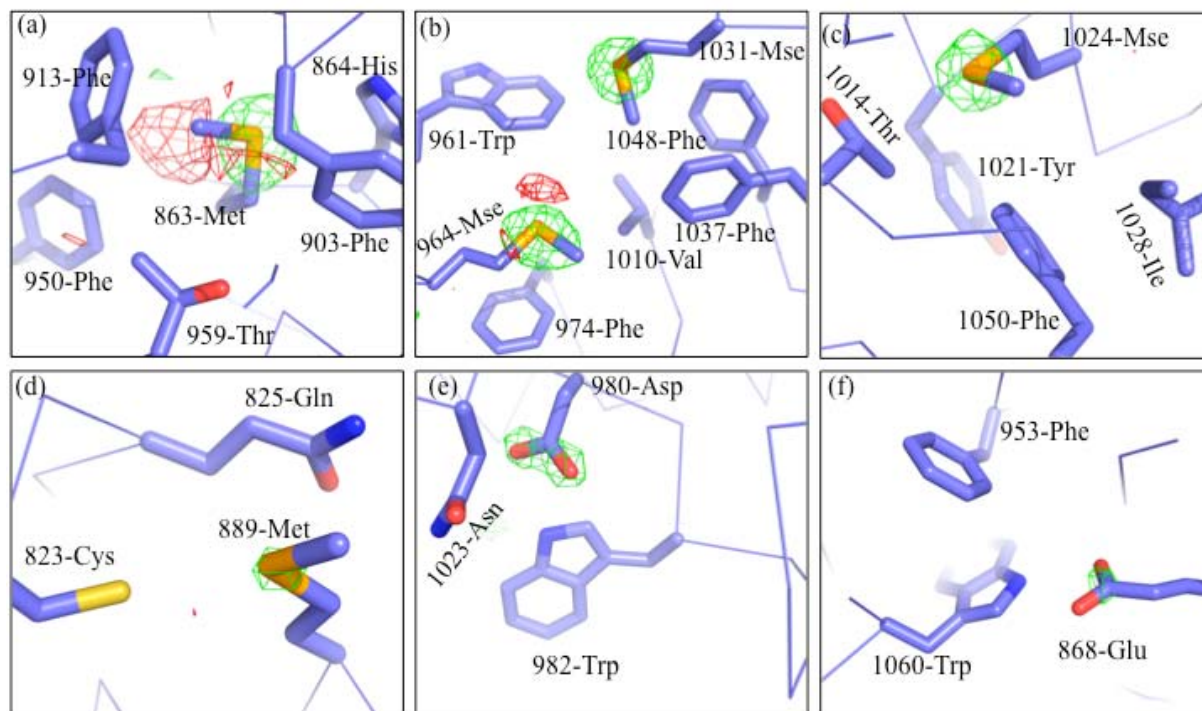


Figure S1. Representative Mse, Glu and Asp residues susceptible to UV radiation in the FAE crystal structure. The positive and negative difference electron density ($F_{before}-F_{after-1}$, Φ_{calc})- maps are shown in green and red at contour level 5σ and -5σ respectively. It is positive where electron density has been lost and negative where it has not been modeled.

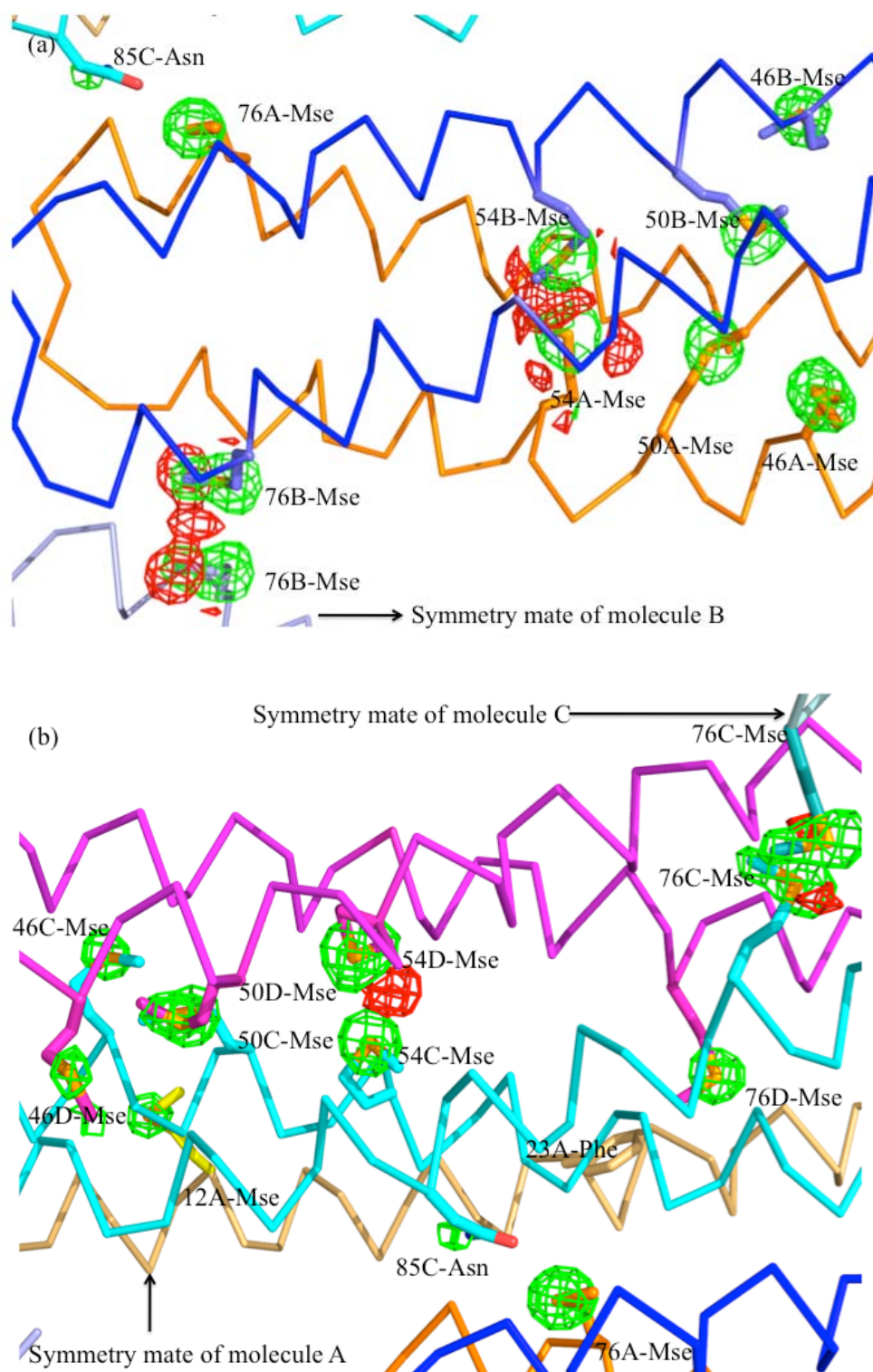


Figure S2. Representative Mse susceptible to UV radiation in the H35 crystal structure. The four C α chains A, B, C and D of the structure are shown in orange, blue, magenta and cyan respectively. The symmetry-related chain of each molecule is shown in the same corresponding color but with reduced darkness. The positive and negative difference electron density ($F_{before} - F_{after-1}$, Φ_{calc})- maps are shown in green and red at contour level 5σ and -5σ respectively.

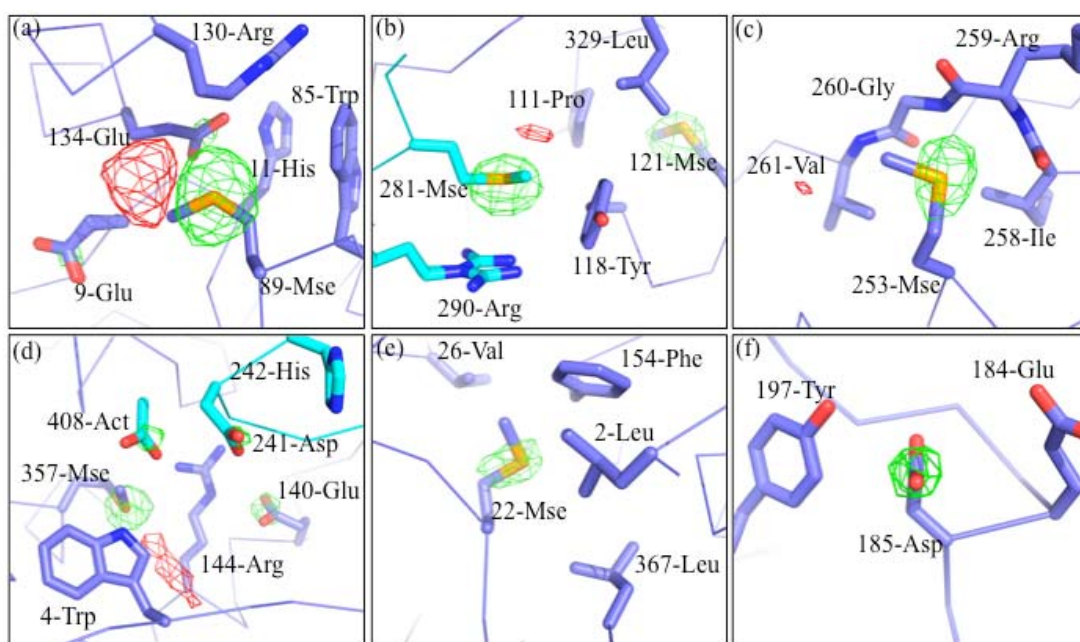


Figure S3. Representative Mse, Glu and Asp residues susceptible to UV radiation in the CHSYNTH crystal structure. The C α chain of the structure and its symmetry related chain are shown in blue and cyan respectively. The positive and negative difference electron density ($F_{before}-F_{after-1}$, Φ_{calc})- maps are shown in green and red at contour level 5σ and -5σ respectively.

Table S1

(a) The peak height of the local maxima and minima of the difference electron density ($F_{before} - F_{after-i} - \Phi_{calc}$)- map in σ (where $i=1$ to 5) for all FAE UV-RIP data identifying the sites at which radiation damage occurs. The second row in the table shows the root mean square (rms) of the difference map. The absolute peak height ($e^{-}/\text{\AA}^3$) is equal to σ multiply of the rms of the difference map. In the bracket, distance (in \AA) from the nearest atom to radiation damage position is provided. The peaks in black font where electron density has been lost and in purple where it has not been modeled.

	after_1	after_2	after_3	after_4	after_5
Rms of the difference map	0.0177	0.0221	0.0263	0.0302	0.0342
Mse-964A-SE	30.57(0.37)	40.77(0.17)	43.40(0.09)	45.68(0.07)	42.95(0.06)
Mse-964B-SE	34.54(0.38)	41.22(0.34)	43.02(0.30)	43.03(0.27)	40.32(0.24)
Mse-863B-SE	38.50(0.09)	43.94(0.07)	41.88(0.07)	40.06(0.07)	37.69(0.06)
Mse-863A-SE	38.50(0.08)	41.68(0.07)	40.73(0.07)	38.73(0.09)	36.81(0.08)
Mse-1031A-SE	19.82(0.23)	26.27(0.19)	28.55(0.14)	30.12(0.14)	30.68(0.13)
Mse-1031B-SE	18.12(0.30)	24.01(0.25)	27.41(0.20)	28.47(0.17)	28.93(0.17)
Mse-1024A-SE	13.02(0.53)	19.48(0.41)	21.32(0.41)	22.51(0.40)	23.67(0.31)
Mse-1024B-SE	11.89(0.48)	16.76(0.30)	19.80(0.26)	21.19(0.24)	22.21(0.25)
Mse-889A-SE	5.66(0.70)	10.87(0.50)	13.69(0.39)	13.90(0.30)	15.49(0.29)
Mse-889B-SE	6.79(0.64)	9.06(0.64)	12.18(0.36)	13.24(0.31)	13.73(0.27)
Mse-975B-SE		6.34(0.42)	8.76(0.42)	10.59(0.40)	12.56(0.37)
Mse-955A-SE	6.79(0.27)	9.06(0.27)	9.52(0.27)	11.26(0.27)	10.81(0.27)
Mse-975A-SE		6.34(0.76)	7.99(0.67)	9.27(0.37)	10.52(0.52)
Mse-946B-SE		6.80(0.52)	7.61(0.52)	7.94(0.52)	10.23(0.50)
Mse-863A-CE	-19.82(1.84)	-18.12(1.84)	-14.85(1.84)	-11.59(1.84)	-9.64(1.84)
Cd-3086A-CD		5.44(0.87)	7.23(0.87)	8.61(0.84)	9.64(0.48)
Cd-3087A-CD	-6.23(0.38)	-7.70(0.38)	-9.14(0.57)	-9.93(0.57)	-9.64(0.57)
Cd-3086B-CD		6.34(0.64)	7.23(0.64)	8.94(0.60)	9.64(0.61)
Mse-946A-SE	6.23(0.73)	6.80(0.73)	8.76(0.17)	9.93(0.14)	9.64(0.13)
Mse-955B-SE		5.89(0.43)	6.85(0.53)	8.61(0.64)	9.35(0.49)
Mse-863B-CE	-18.68(1.51)	-15.86(1.51)	-13.32(1.51)	-10.92(1.51)	-9.06(1.51)
Asp-980B-OD1	7.93(0.40)	9.06(0.41)	9.14(0.40)	9.27(0.40)	8.47(0.40)
Cd-3089A-CD		-5.89(0.51)	-6.47(0.81)	-6.29(0.51)	-7.60(0.81)
His-1084B-NE2		-5.89(1.68)	-6.47(1.68)	-6.62(1.60)	-7.60(1.68)
Asp-980A-OD1		7.70(0.51)	8.76(0.37)	8.61(0.34)	7.60(0.32)
Cd-3087B-CD	-5.66(0.21)	-5.44(0.50)	-6.47(0.59)	-7.28(0.59)	-7.30(0.59)
Cd-3089B-CD		-5.89(0.73)	-6.85(0.79)	-6.95(0.79)	-6.72(0.79)
Asp-1018B-OD1			5.33(0.38)	4.97(0.38)	6.14(0.38)
Mse-964A-C				6.62(0.80)	6.14(0.80)
Mse-964A-CG	-5.66(1.76)	-6.80(1.76)	-6.47(1.76)	-5.96(1.80)	-6.14(1.76)
Glu-868B-CD	5.66(0.24)	5.44(0.72)	5.71(0.86)	5.63(0.66)	6.14(0.66)
Mse-964A-CB			-5.33(1.34)	-5.96(1.65)	-5.84(1.65)
Cd-3088B-CD		-6.80(0.83)	-6.47(0.15)	-5.30(0.15)	-5.84(0.15)
Mse-964B-CB	-5.10(0.60)	-5.89(1.01)	-6.47(1.01)	-5.96(1.01)	-5.84(1.01)
Glu-868A-CD				5.96(0.15)	5.55(0.15)
Tyr-1066A-OH					5.55(0.31)
Lys-990B-NZ				5.30(0.69)	5.55(0.45)
Sep-954A-OIP				-5.30(0.66)	-5.55(0.66)
Tyr-1008A-CD1		-5.89(1.47)	-5.33(1.47)	-5.30(1.47)	-5.55(1.47)
Gln-1027A-OE1			6.09(0.33)	5.63(0.33)	5.26(0.33)
Gly-979B-C				4.97(0.61)	5.26(0.61)
Val-963B-O				-5.30(0.92)	-5.26(1.12)
Mse-863A-CA	-5.66(1.33)	-5.44(1.33)	-5.71(1.33)	-5.30(1.33)	-5.26(1.33)
Pro-901A-O					-5.26(1.59)
Mse-964B-CG		4.98(0.90)	4.95(0.90)	5.30(0.90)	5.26(0.87)
Wat-2324A-O		4.98(0.19)	4.95(0.19)	5.30(0.19)	5.26(0.19)
Glu-916B-CD					4.97(0.28)
Cys-967B-SG		5.44(0.59)	4.95(0.59)	4.97(0.59)	4.97(0.59)
Mse-975B-CE					4.97(0.62)
Wat-2192B-O					-4.97(1.49)
Mse-1031B-CG					-4.97(1.84)
Glu-916A-OE1					4.97(0.57)
Number of positive peaks	14	24	26	30	33
Number of negative peaks	7	12	13	15	19

(b): The peak height of the local maxima and minima of the difference electron density ($F_{before} - F_{after-i}$, Φ_{calc})- map in σ (where $i=1$ to 5) for all H35 UV-RIP data identifying the sites at which radiation damage occurs.

	after-1	after-2	after-3	after-4	after-5
Rms of the difference map	0.0183193	0.0228595	0.0259197	0.028498	0.030927
Mse-54A-SE	40.94(0.26)	35.87(0.24)	32.41(0.21)	31.23(0.18)	29.42(0.20)
Mse-54A-SE	-15.28(1.86)	-15.31(1.86)	-15.05(1.86)	-13.69(1.86)	-12.93(1.86)
Mse-54B-SE	27.29(0.29)	27.12(0.22)	27.01(0.19)	26.32(0.18)	25.87(0.17)
Mse-50A-SE	15.28(0.37)	18.37(0.37)	20.06(0.37)	20.35(0.36)	21.02(0.37)
Mse-50B-SE	13.10(0.41)	15.75(0.35)	16.98(0.32)	16.84(0.26)	18.43(0.29)
Mse-76B-CE	16.92(0.15)	17.94(0.15)	18.52(0.14)	17.90(0.12)	18.11(0.57)
Mse-54D-SE	19.65(0.52)	18.37(0.48)	18.90(0.46)	18.60(0.15)	17.78(0.15)
Mse-54C-SE	13.10(0.35)	15.75(0.35)	16.20(0.35)	16.84(0.35)	16.49(0.29)
Mse-46A-SE	12.56(0.33)	14.44(0.33)	14.66(0.33)	15.09(0.32)	14.55(0.33)
Mse-50C-SE	9.28(0.46)	11.37(0.46)	12.73(0.46)	12.63(0.41)	12.61(0.39)
Mse-76A-SE	7.64(0.67)	10.06(0.67)	10.80(0.65)	10.88(0.55)	11.64(0.18)
Mse-19B-SE	11.46(0.60)	10.94(0.38)	12.35(0.33)	11.23(0.38)	11.32(0.32)
Mse-76C-SE	7.10(0.18)	8.75(0.18)	9.65(0.18)	10.88(0.18)	10.99(0.18)
Mse-46B-SE	6.00(0.59)	7.87(0.59)	9.26(0.59)	9.83(0.30)	10.35(0.26)
Mse-46B-SE	-16.92(2.58)	-13.12(2.58)	-11.57(2.58)	-10.53(2.58)	-10.35(2.58)
Mse-50D-CE	7.64(0.50)	8.75(0.50)	10.03(0.50)	9.47(0.50)	9.70(0.52)
Mse-46C-SE	6.00(0.15)	7.44(0.66)	8.87(0.15)	8.77(0.15)	9.38(0.15)
Mse-54A-CE	-9.28(2.15)	-10.06(2.15)	-10.03(2.15)	-9.12(2.62)	-9.38(2.15)
Val-94C-CG1	6.55(0.77)	8.31(0.75)	8.49(0.75)	7.72(0.77)	8.08(0.76)
Mse-34D-SE		5.69(0.36)	6.94(0.35)	7.37(0.74)	7.76(0.32)
Mse-76B-SE	-8.73(2.58)	-8.31(2.58)	-7.33(2.58)	-7.37(2.58)	-7.44(2.58)
Mse-19C-SE	5.46(0.69)	6.12(0.86)	6.56(0.54)	7.02(0.54)	7.11(0.80)
Mse-12A-SE			5.02(0.74)	6.67(0.30)	6.79(0.30)
Mse-19D-SE	5.46(0.56)	6.56(0.56)	6.94(0.51)	6.32(0.60)	6.79(0.40)
Mse-34B-SE		5.25(0.57)	6.17(0.57)	6.32(0.57)	6.47(0.57)
Mse-12C-SE	6.00(0.48)	6.12(0.48)	6.56(0.48)	6.67(0.48)	6.47(0.48)
Mse-76D-SE			5.02(1.07)	5.97(0.49)	6.47(0.49)
Mse-50B-SE	-6.00(2.60)	-6.56(2.59)	-7.72(2.59)	-7.02(2.59)	-6.14(2.58)
Mse-50B-SE				-5.61(2.15)	-6.14(2.14)
Mse-12C-SE			5.79(0.04)	5.97(0.04)	6.14(0.04)
Mse-54A-SE	-10.92(2.40)	-8.75(2.45)	-6.94(2.45)	-6.32(2.45)	-6.14(2.45)
Mse-50A-CB					-6.14(1.76)
Mse-19D-SE	5.46(0.56)	6.56(0.56)	6.94(0.51)	6.32(0.60)	5.50(0.60)
Mse-50B-CG		-5.25(1.94)	-5.02(1.94)	-5.26(1.94)	-5.50(1.94)
Mse-46D-SE			5.02(0.37)	5.26(0.37)	5.50(0.37)
Mse-12D-SE				5.26(0.85)	5.17(0.93)
Mse-76C-SE		-4.37(2.17)	-5.02(2.17)	-5.26(2.17)	-5.17(2.17)
Mse-76B-CB		-4.37(1.89)	-4.63(1.89)	-4.91(1.89)	-5.17(1.89)
Number of positive peaks	20	22	26	27	27
Number of negative peaks	6	9	9	10	11

(c): The peak height of the local maxima and minima of the difference electron density ($F_{before} - F_{after-i}$ Φ_{calc}) - map in σ (where $i=1$ to 5) for all CHSYNTH UV-RIP data identifying the sites at which radiation damage occurs.

	after-1	after-2	after-3	after-4	after-5
Rms of the difference map	0.0099326	0.0125922	0.0148707	0.0170443	0.0191158
Mse-A89-SE	36.24(0.38)	38.12(0.36)	36.99(0.35)	35.79(0.33)	32.43(0.33)
Mse-A121-SE	16.11(0.77)	20.65(0.77)	22.86(0.76)	22.29(0.76)	21.97(0.76)
Mse-A281-SE	21.14(0.99)	23.03(0.28)	22.86(0.25)	22.29(0.24)	21.97(0.26)
Mse-A253-SE	13.09(0.56)	16.68(0.56)	18.16(0.56)	18.77(0.56)	19.36(0.56)
Mse-A357-SE	15.10(0.39)	17.47(0.39)	18.16(0.66)	17.60(0.62)	18.83(0.58)
Mse-A22-SE	11.07(0.34)	15.88(0.34)	16.14(0.34)	17.60(0.34)	16.74(0.34)
Mse-A89-SE	-20.14(2.71)	-16.68(2.71)	-13.45(2.71)	-12.91(2.71)	-12.56(2.71)
Asp-A373-OD2	8.05(0.48)	11.12(0.48)	11.43(0.48)	11.73(0.48)	12.03(0.48)
Glu-A134-OE2	7.05(0.86)	9.53(0.49)	9.41(0.49)	8.80(0.48)	9.94(0.49)
Glu-A140-OE1	9.06(0.70)	11.12(0.70)	10.09(0.70)	9.97(0.70)	9.94(0.70)
Act-A408-C	8.05(0.43)	9.53(0.43)	10.76(0.43)	9.97(0.43)	9.94(0.43)
Glu-A9-CD	8.05(0.21)	9.53(0.21)	10.09(0.21)	10.56(0.21)	9.42(0.21)
Mse-A302-SE		6.35(0.33)	8.07(0.33)	7.63(0.33)	9.42(0.33)
Asp-A185-CG	7.05(0.48)	7.94(0.48)	8.07(0.80)	8.21(0.55)	8.89(0.76)
Thr-A6-CB	5.03(0.95)	7.94(0.79)	8.07(0.79)	7.63(0.79)	7.85(0.79)
Asp-A241-CG	7.05(0.45)	8.74(0.45)	8.74(0.45)	8.21(0.45)	7.85(0.82)
Wat-A618-O	-6.04(2.15)	-5.56(2.15)	-6.72(2.15)	-7.04(2.15)	-7.85(2.15)
Glu-A224-CD	6.04(0.52)	7.15(0.38)	8.07(0.38)	7.04(0.65)	7.32(0.61)
Val-A261-CB	-7.05(2.96)	-7.15(2.96)	-6.72(2.96)	-6.45(2.96)	-7.32(2.96)
Glu-A280-CD					6.80(0.60)
Ser-A236-CB	7.15(0.73)	7.15(0.73)	6.72(0.45)	5.87(0.74)	6.28(0.90)
Lys-A259-NZ	5.03(3.21)	6.35(3.21)	6.72(3.21)	6.55(3.21)	6.28(3.21)
Glu-A9-CG		-6.35(1.87)	-6.72(1.87)	-7.04(2.67)	-6.28(2.55)
His-A242-CE1		5.56(0.64)	6.72(0.64)	6.45(0.64)	6.28(0.64)
HOH-A679-O	6.04(2.71)	5.56(2.71)	5.38(2.71)	6.45(2.71)	6.28(2.71)
Tyr-A197-CZ					6.28(0.61)
Mse-A357-SE	-8.05(3.07)	-7.15(3.07)	-6.72(3.07)	-6.55(3.07)	-6.28(3.07)
Asp-A241-OD1				-5.87(2.30)	-6.28(2.30)
Mse-A253-CB	-5.03(1.82)	-6.35(1.82)	-7.40(1.82)	-5.87(1.82)	-6.28(1.82)
Leu-A367-CD1	-5.03(2.50)	-7.15(2.50)	-5.38(2.50)	-6.45(2.30)	-6.28(2.50)
Gly-A70-O			-6.05(2.23)	-5.28(2.23)	-6.28(2.23)
Asp-A9-CG		-6.35(1.87)	-6.72(1.87)	-7.04(2.67)	-6.28(2.55)
Thr-A6-CG2	-7.05(3.13)	-6.35(2.41)	-6.72(2.41)	-7.63(2.41)	-5.75(2.41)
Asp-A215-OD1		5.56(0.39)	6.05(0.39)	5.28(1.07)	5.75(0.86)
Glu-A368-CD	6.04(0.64)	6.35(0.64)	6.05(0.64)	7.63(0.64)	5.75(1.12)
Glu-A299-CD			6.72(0.55)	5.87(0.55)	5.75(0.55)
Pro-A113-CA					-5.75(2.61)
Mse-A314-CB				-5.28(2.41)	-5.75(2.41)
HOH-A683-O	5.03(0.91)	7.15(0.91)	7.40(0.91)	7.04(0.91)	5.75(0.91)
Glu-A377-CD				5.28(0.66)	5.75(0.66)
Arg-A130-NH1					-5.75(2.12)
Leu-A164-O	-5.03(1.50)	-5.93(1.50)	-6.72(1.50)	-5.28(1.50)	-5.75(1.50)
Leu-A15-CD2		-6.35(1.41)	-6.05(1.41)	-5.95(1.41)	-5.75(1.41)
HOH-A646-O	6.04(0.72)	5.88(0.72)	5.38(0.80)	5.28(0.52)	5.75(0.80)
Asp-A245-CG			6.72(0.82)	5.87(0.82)	5.75(0.24)
Mse-A281-CE	-7.05(2.27)	-6.35(2.27)	-6.72(2.33)	-5.87(2.27)	-5.75(2.56)
Ile-A75-CD1			-5.38(3.08)	-5.87(3.08)	-5.75(3.08)
Glu-A262-CD				5.87(0.20)	5.23(0.20)
His-A11-CB					-5.23(2.26)
Lys-A123-NZ	6.04(1.75)	5.56(1.75)	5.38(2.53)	5.28(2.53)	5.23(2.53)
Ser-A61-OG		6.35(0.55)	5.38(0.36)	5.87(0.55)	5.23(0.55)
Thr-A326-OG1		-5.56(2.47)	-4.71(2.47)	-5.28(2.47)	-5.23(2.47)
Mse-A253-SE	-5.03(2.19)	-6.35(2.10)	-6.72(2.19)	-6.45(2.19)	-5.23(2.13)
Thr-A6-CG2	-7.05(3.13)	-6.35(2.41)	-6.72(2.41)	-7.63(2.41)	-5.75(2.41)
Mse-A121-CE		-4.76(2.19)	-5.02(2.19)	-5.28(2.19)	-5.23(2.19)
Wat-A667-O	5.03(0.63)	7.94(0.36)	6.05(0.63)	7.04(0.36)	5.23(0.56)
Asp-A241-OD2		-4.76(2.07)	-5.02(2.07)	-5.28(2.07)	-5.23(2.07)
Asp-A117-OD1					-5.23(2.27)
Val-A94-CG2					5.23(1.23)
Act-A408-OXT					-5.23(2.62)
Tyr-A124-OH	-5.03(2.29)	-5.56(2.29)	-5.38(2.29)	-5.87(2.29)	-5.23(2.29)
HOH-A629-O					-5.23(2.43)
Arg-A243-NH1					-5.23(1.85)

Number of positive peaks	23	27	27	29	30
Number of negative peaks	12	18	20	21	28