The Polarizable Atomic Multipole-based AMOEBA Force Field for Proteins

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Table S1. Electrostatic dipole moments for individual amino acids. The permanent atomic multipoles (PAMs) were derived from the specified model compounds. Dipeptide molecular dipole moments of the conformations from the validation set are listed here. The corresponding ϕ and ψ angles can be found in Table S2.

	Dipeptide Dipole Moments (debye) AMOEBA vs MP2/aug-cc-pVTZ (parenthesis)			
	Dx	**Dy**	**Dz**	**Dtotal**
Cys	-1.32(-1.30)	-2.28(-2.21)	0.33(0.31)	2.66(2.59)
	2.63(2.70)	-0.94(-0.81)	1.28(1.41)	3.07(3.15)
	-3.27(-3.18)	-1.16(-1.11)	0.12(0.14)	3.47(3.37)
Met	1.59(1.64)	-1.61(-1.72)	2.04(1.82)	3.05(3.00)
	-1.72(-1.68)	-2.76(-2.76)	-0.31(-0.41)	3.27(3.27)
	2.25(2.18)	-0.71(-0.57)	1.31(1.43)	2.70(2.66)
Ser	-3.47 (-3.45)	0.31 (0.37)	-2.06 (-2.09)	4.05(4.05)
	-4.47(-4.31)	-2.07(-1.90)	-2.42(-2.44)	5.49(5.30)
	2.75(2.97)	-1.98(-1.85)	-0.56(-0.49)	3.43(3.54)
Thr	-0.11(-0.12)	1.81(1.63)	-0.24(-0.17)	1.83(1.65)
	1.68(1.58)	0.02(0.26)	0.19(0.20)	1.69(1.62)
	1.79(1.73)	0.14(0.41)	0.30(0.35)	1.82(1.82)
His	8.57(8.50)	-4.62(-4.96)	-0.32(-0.39)	9.74(9.85)
	11.94(11.18)	-4.70(-4.58)	-4.40(-3.89)	13.56(12.69)
	5.34(5.44)	0.89(0.63)	-1.36(-1.23)	5.59(5.62)
Hid	-4.34(-4.37)	-4.21(-4.27)	-0.13(-0.19)	6.04(6.11)
	5.61(5.59)	-0.22(0.01)	1.43(1.47)	5.80(5.78)
	3.44(3.18)	0.05(-0.13)	0.27(0.11)	3.45(3.19)
Hie	-2.59(-2.91)	5.36(5.20)	-2.54(2.47)	6.47(6.45)
	7.37(7.55)	-3.69(-3.74)	-0.05(-0.06)	8.24(8.43)
	-1.63(-1.84)	0.51(0.43)	-3.60(-3.62)	3.98(4.08)
Leu	-0.71(-0.76)	2.32(2.23)	-0.85(-0.97)	2.58(2.55)
	2.09(2.42)	-1.69(-1.62)	-0.07(-0.09)	2.68(2.92)
	0.86(0.84)	-1.66(-1.65)	0.33(0.43)	1.90(1.90)
Ile	2.71(2.86)	-0.23(-0.23)	-0.25(-0.25)	2.73(2.88)
	-1.18(-1.20)	-1.56(-1.47)	-0.20(-0.29)	1.96(1.92)
	-0.15(-0.06)	-2.45(-2.44)	-1.41(-1.48)	2.84(2.85)
Val	-1.05(-0.92)	-1.74(-1.67)	-0.48(-0.70)	2.09(2.03)
	1.11(1.00)	-1.57(-1.60)	0.43(0.55)	1.97(1.96)
	1.02(1.22)	-3.48(-3.62)	4.53(4.45)	5.80(5.89)
Phe	2.32(2.61)	2.21(2.05)	1.37(1.44)	3.49(3.61)
	-0.44(-0.38)	2.38(2.26)	-0.60(-0.75)	2.49(2.41)
	1.06(0.99)	2.22(2.04)	1.15(1.24)	2.73(2.58)

Tyr	-1.14(-1.08)	0.07(0.04)	-1.83(-1.71)	2.16(2.02)
	-0.93(-1.22)	1.24(1.06)	-1.42(1.46)	2.10(2.18)
	-2.50(-2.73)	2.19(2.21)	0.68(0.81)	3.40(3.61)
Trp	-5.66(-5.98)	-0.87(-0.95)	-3.00(2.98)	6.47(6.75)
	3.60(3.72)	1.12(1.27)	2.29(2.23)	4.42(4.52)
	-2.08(-2.21)	-0.01(-0.22)	-2.07(-2.09)	2.93(3.05)
Arg	-11.23(-11.13)	-2.14(-1.98)	2.88(2.88)	11.79(11.67)
	7.45(7.56)	3.34(2.80)	-1.58(-1.21)	8.32(8.16)
	11.76(11.45)	-3.00(-2.96)	-3.07(-2.97)	12.51(12.19)
Asp	4.19(4.46)	0.25(0.40)	1.46(1.74)	4.44(4.80)
	-4.64(-4.82)	-7.61(-8.16)	1.65(1.54)	9.06(9.60)
	-10.96(-11.37)	1.34(1.31)	-6.27(-6.30)	12.70(12.70)
Asph	3.33(3.45)	-6.24(-5.56)	0.10(-0.23)	7.08(6.55)
	-5.98(-5.60)	-1.88(-2.38)	-2.76(-3.02)	6.85(6.79)
	5.12(4.65)	3.00(2.87)	-6.47(-6.50)	8.78(8.49)
Asn	-0.58(-0.47)	0.07(-0.04)	2.74(2.39)	2.80(2.44)
	-3.63(-3.85)	-0.57(-0.64)	-2.59(2.51)	4.50(4.64)
	-1.70(-1.98)	0.19(-0.02)	-6.99(-6.79)	7.20(7.07)
Glu	-5.00(-4.69)	-0.22(-0.46)	0.04(0.29)	5.00(4.72)
	15.69(16.07)	-0.89(-1.01)	3.25(3.27)	16.04(16.43)
	15.08(15.24)	-0.47(-0.54)	0.62(0.47)	15.10(15.26)
Gln	2.71(2.74)	-0.36(-0.50)	-4.61(-4.47)	5.36(5.27)
	-4.46(-4.72)	-1.21(-1.35)	-5.14(-4.84)	6.91(6.90)
	-0.93(-1.02)	3.69(3.80)	2.91(2.84)	4.79(4.85)
Lys	-11.54(-11.20)	0.25(0.07)	2.93(2.86)	11.91(11.56)
	17.19(17.24)	0.83(1.00)	1.12(1.11)	17.24(17.31)
	13.40(13.46)	0.90(0.97)	-3.01(-2.99)	13.76(13.82)

Table S2. The RMSE (kcal/mol per charge unit) between AMOEBA and *ab initio* (MP2/aug-cc-pVTZ) electrostatic potentials. The RMSE values for all conformers of each model compound are listed.

		Parameterization set					Validation set
		α_L	α'	C5	C7*a*	C7*e*	β2
Ala	ϕ	63.50	-166.10	-158.40	73.90	-82.90	-137.90
	ψ	34.80	-37.20	161.30	-64.00	77.90	22.90
	RMSE	0.40	0.43	0.35	0.28	0.32	0.46

		Parameterization set	Validation set
Pro	ϕ	40.00	-85.70
	ψ	55.00	74.00
	RMSE	0.27	0.29

		Parameterization set		Validation set
Gly	ϕ	-83.00	172.30	-90.00
	ψ	74.70	177.00	180.00
	RMSE	0.14	0.16	0.18

	Ala-NH_3	Ala-COOH	Ala-COO	Ala-NH_2	Gly-NH_3	Gly-COOH
RMSE	0.39	0.39	0.57	0.58	0.22	0.58

		Parameterization set			Validation set		
Cys	ϕ	-140.41	-140.41	-87.24	-87.24	-87.24	-140.41
	ψ	159.78	159.78	81.12	81.12	81.12	159.78
	χ	0.00	150.00	-30.00	60.00	-150.00	-90.00
	RMSE	0.28	0.27	0.32	0.32	0.40	0.38
Met	ϕ	-75.12	-93.37	-131.24	-82.28	-85.25	-82.28
	ψ	-26.89	0.52	18.04	79.49	64.39	79.49
	χ	-175.10	-72.90	-62.50	-170.80	-150.00	-170.00
	RMSE	0.43	0.41	0.36	0.40	0.33	0.32
Ser	ϕ	-76.13	-156.36	-84.63	-84.62	75.44	-173.55
	ψ	-20.69	-171.94	66.55	66.56	-37.77	168.89
	χ	-51.40	-168.30	179.90	179.00	84.40	-92.80
	RMSE	0.80	0.61	0.59	0.59	0.41	0.67
Thr	ϕ	-82.40	-70.71	-101.99	-82.39	-154.91	-155.67

	ψ	78.05	-30.42	137.96	78.04	-178.26	-177.30
	χ	-66.20	-170.60	-175.80	-66.20	71.70	69.20
	RMSE	0.41	0.48	0.52	0.41	0.46	0.47
His	ϕ	-158.24	-124.68	51.48	-140.00	-60.00	-161.76
	ψ	27.69	136.26	48.61	135.00	-45.00	37.48
	χ	156.20	-59.90	-62.50	-60.00	60.00	-117.74
	RMSE	0.64	0.55	0.49	0.55	1.19	0.47
Hid	ϕ	-79.05	-119.62	-83.85	-83.85	-83.85	-83.85
	ψ	-18.18	17.74	73.71	73.71	73.71	73.71
	χ	-169.00	-89.00	170.00	171.62	31.53	-172.00
	RMSE	0.57	0.42	0.34	0.34	0.44	0.59
Hie	ϕ	-68.05	-80.38	-156.70	-83.49	-156.70	-83.49
	ψ	-35.58	-17.06	-156.10	51.82	-156.10	51.82
	χ	-172.92	-59.12	150.00	54.80	69.10	54.80
	RMSE	0.54	0.57	0.50	0.53	0.51	0.40
Leu	ϕ	-124.77	-72.96	-82.47	-83.81	-155.58	-81.06
	ψ	15.28	-30.83	83.56	79.25	143.66	85.83
	χ	-59.30	179.0	-177.70	-55.40	120.0	-178.1
	RMSE	0.32	0.42	0.29	0.35	0.48	0.32
Ile	ϕ	-72.10	-130.00	-84.13	-151.81	-82.19	-84.86
	ψ	-35.05	132.96	68.47	156.22	83.40	59.73
	χ	-69.90	-58.90	52.30	-168.20	179.20	54.30
	RMSE	0.36	0.38	0.30	0.29	0.32	0.33
Val	ϕ	-71.27	-131.52	-132.55	-85.60	-85.60	-77.60
	ψ	-34.77	134.41	165.37	88.90	88.90	-32.20
	χ	-65.90	-57.40	63.60	-120.00	-180.00	150.00
	RMSE	0.41	0.34	0.28	0.46	0.48	0.51
Phe	ϕ	-67.20	-159.33	-78.56	-80.60	-84.17	-87.05
	ψ	-38.86	173.79	-19.59	41.63	76.28	74.43
	χ	178.90	120.00	-57.00	0.00	-77.20	-66.20
	RMSE	0.49	0.31	0.48	0.51	0.42	0.36
Tyr	ϕ	-66.82	-78.61	-161.31	70.56	-83.84	-161.38
	ψ	-39.10	-19.71	151.48	38.42	53.64	151.48
	χ	-79.40	-57.10	178.30	-62.60	44.00	-178.20
	RMSE	0.51	0.46	0.34	0.65	0.46	0.38
Trp	ϕ	-69.06	-78.43	-83.98	-60.00	-60.00	-140.00
	ψ	-37.71	-19.89	54.64	-45.00	-45.00	135.00
	χ	174.90	-55.40	49.30	60.00	-90.00	-179.40
	RMSE	0.55	0.49	0.49	0.54	0.49	0.53
Arg	ϕ	-148.86	-77.57	-85.33	-77.57	-85.33	-157.03
	ψ	37.42	-20.65	68.93	-20.65	68.93	35.71
	χ	-60.80	173.10	61.40	173.10	60.00	-152.50

	RMSE	0.56	0.63	0.66	0.63	0.66	1.09
Asp	ϕ	-70.55	-84.50	-155.44	-60.00	-140.00	-60.00
	ψ	-30.13	-24.50	171.95	-45.00	135.00	-45.00
	χ	-51.75	-162.42	-166.14	60.00	-160.00	-177.58
	RMSE	0.52	0.59	0.73	0.58	0.80	0.49
Asph	ϕ	-144.60	-79.22	-83.38	-140.00	-60.00	-60.00
	ψ	24.86	-17.20	73.60	135.00	-45.00	-45.00
	χ	-56.80	-58.90	-174.40	60.00	150.00	-90.00
	RMSE	0.43	0.49	0.40	1.08	1.15	0.92
Asn	ϕ	-79.61	-84.03	-83.95	-140.00	-60.03	-60.00
	ψ	-16.43	59.40	57.60	135.00	-44.29	-45.00
	χ	-59.10	-50.90	51.50	-174.80	-53.10	-45.00
	RMSE	0.53	0.43	0.43	0.76	0.53	0.66
Glu	ϕ	-88.43	-93.86	-67.30	-60.00	-60.00	-140.00
	ψ	-15.44	-4.90	-38.92	-45.00	-45.00	135.00
	χ	-57.38	80.59	-179.44	60.00	-177.70	-90.00
	RMSE	0.65	0.76	0.49	0.95	0.57	0.62
Gln	ϕ	-130.02	-157.43	-75.02	-60.00	-60.00	-140.00
	ψ	16.19	175.05	-26.26	-45.00	-45.00	135.00
	χ	-65.77	-104.15	-173.82	60.00	176.50	120.00
	RMSE	0.41	0.45	0.65	0.56	0.75	0.50
Lys	ϕ	-148.74	-84.82	-152.99	-83.23	-157.41	-83.73
	ψ	35.58	74.53	25.53	61.15	34.54	76.51
	χ	-166.93	-161.43	-149.24	-65.39	-163.91	-165.80
	RMSE	0.59	0.67	0.45	0.72	0.54	0.50

Table S3. HA-CA-CB-HB *J*-Coupling data (Hz) for BPTI.

Residue index	Dihedral angle	*J*-expt.	*J*-calc.
PHE-4	4_HA_4_CA_4_CB_4_2HB	4.5	4.04
PHE-4	4_HA_4_CA_4_CB_4_HB3	4.5	3.81
CYS-5	5_HA_5_CA_5_CB_5_HB3	3.0	2.86
CYS-5	5_HA_5_CA_5_CB_5_2HB	12.0	10.09
THR-11	11_HA_11_CA_11_CB_11_HB	8.2	9.17
CYS-14	14_HA_14_CA_14_CB_14_HB3	3.0	2.34
CYS-14	14_HA_14_CA_14_CB_14_2HB	12.0	10.09
LYS-15	15_HA_15_CA_15_CB_15_HB3	3.5	5.08
LYS-15	15_HA_15_CA_15_CB_15_2HB	11.0	9.17
ILE-18	18_HA_18_CA_18_CB_18_HB	10.5	10.00
ILE-19	19_HA_19_CA_19_CB_19_HB	11.0	10.01
ARG-20	20_HA_20_CA_20_CB_20_HB3	2.5	2.93
ARG-20	20_HA_20_CA_20_CB_20_2HB	12.5	10.83
PHE-22	22_HA_22_CA_22_CB_22_HB3	3.5	2.63
PHE-22	22_HA_22_CA_22_CB_22_2HB	4.4	5.74
TYR-23	23_HA_23_CA_23_CB_23_HB3	12.5	10.77
TYR-23	23_HA_23_CA_23_CB_23_2HB	3.8	4.20
ASN-24	24_HA_24_CA_24_CB_24_HB3	12.0	8.17
ASN-24	24_HA_24_CA_24_CB_24_2HB	3.5	4.41
CYS-30	30_HA_30_CA_30_CB_30_2HB	12.0	10.03
CYS-30	30_HA_30_CA_30_CB_30_HB3	2.5	2.22
GLN-31	31_HA_31_CA_31_CB_31_HB3	3.5	3.58
GLN-31	31_HA_31_CA_31_CB_31_2HB	11.0	10.44
THR-32	32_HA_32_CA_32_CB_32_HB	2.5	5.70
PHE-33	33_HA_33_CA_33_CB_33_HB3	3.0	2.59
PHE-33	33_HA_33_CA_33_CB_33_2HB	4.5	5.98
VAL-34	34_HA_34_CA_34_CB_34_HB	10.5	9.95
TYR-35	35_HA_35_CA_35_CB_35_HB3	11.5	10.50
TYR-35	35_HA_35_CA_35_CB_35_2HB	6.5	2.87
CYS-38	38_HA_38_CA_38_CB_38_2HB	6.5	3.60
CYS-38	38_HA_38_CA_38_CB_38_HB3	1.5	2.83
LYS-41	41_HA_41_CA_41_CB_41_HB3	2.5	3.46
LYS-41	41_HA_41_CA_41_CB_41_2HB	12.5	10.67
ASN-43	43_HA_43_CA_43_CB_43_2HB	3.0	2.81
ASN-43	43_HA_43_CA_43_CB_43_HB3	12.0	10.53
ASN-44	44_HA_44_CA_44_CB_44_2HB	4.0	4.19
ASN-44	44_HA_44_CA_44_CB_44_HB3	11.0	10.42
PHE-45	45_HA_45_CA_45_CB_45_HB3	4.0	4.21

PHE-45	45_HA_45_CA_45_CB_45_2HB	11.8	10.55
LYS-46	46_HA_46_CA_46_CB_46_HB3	4.0	6.55
LYS-46	46_HA_46_CA_46_CB_46_2HB	9.5	6.72
SER-47	47_HA_47_CA_47_CB_47_2HB	3.0	8.41
SER-47	47_HA_47_CA_47_CB_47_HB3	2.8	2.90
CYS-51	51_HA_51_CA_51_CB_51_HB3	11.5	10.07
CYS-51	51_HA_51_CA_51_CB_51_2HB	5.5	2.81
MET-52	52_HA_52_CA_52_CB_52_2HB	3.0	5.01
MET-52	52_HA_52_CA_52_CB_52_HB3	10.2	8.70
THR-54	54_HA_54_CA_54_CB_54_HB	10.0	9.18
CYS-55	55_HA_55_CA_55_CB_55_2HB	11.0	10.14
CYS-55	55_HA_55_CA_55_CB_55_HB3	1.5	2.55

Table S4. HA-CA-CB-HB *J*-coupling data for GB3 domain.

Residue index	Dihedral angle	*J*-expt.	*J*-calc.
TYR-3	HA_CA_CB_HB2	11.8	10.75
TYR-3	HA_CA_CB_HB3	1.9	3.33
ASN-8	HA_CA_CB_HB2	6.0	3.03
ASN-8	HA_CA_CB_HB3	7.0	10.63
ASP-22	HA_CA_CB_HB2	4.0	5.12
ASP-22	HA_CA_CB_HB3	2.1	4.70
PHE-30	HA_CA_CB_HB2	11.3	10.47
PHE-30	HA_CA_CB_HB3	0.8	4.12
ASN-35	HA_CA_CB_HB2	7.9	3.43
ASN-35	HA_CA_CB_HB3	7.2	10.74
ASN-37	HA_CA_CB_HB2	12.3	10.73
ASN-37	HA_CA_CB_HB3	1.9	3.16
ASP-40	HA_CA_CB_HB2	3.6	3.72
ASP-40	HA_CA_CB_HB3	10.2	10.59
TRP-43	HA_CA_CB_HB2	11.1	8.60
TRP-43	HA_CA_CB_HB3	1.8	3.95
TYR-45	HA_CA_CB_HB2	4.4	3.61
TYR-45	HA_CA_CB_HB3	11.2	10.75
ASP-46	HA_CA_CB_HB2	3.4	4.61
ASP-46	HA_CA_CB_HB3	11.8	8.43
ASP-47	HA_CA_CB_HB2	3.6	4.05
ASP-47	HA_CA_CB_HB3	11.1	10.28

Table S5. N/C'-CA-CB-CG *J*-coupling data for GB3 domain.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
VAL-6	VAL_NCG2	0.5	0.90
VAL-6	VAL_CCG1	0.7	0.57
VAL-6	VAL_NCG1	2.0	2.08
VAL-6	VAL_CCG2	3.7	4.05
ILE-7	ILE_CCG2	0.6	3.91
ILE-7	ILE_NCG2	2.0	1.25
THR-11	THR_NCG2	0.9	1.53
THR-11	THR_CCG2	2.1	0.22
THR-16	THR_NCG2	0.2	1.54
THR-16	THR_CCG2	1.8	0.28
THR-17	THR_NCG2	0.6	0.67
THR-17	THR_CCG2	2.8	3.39
THR-18	THR_NCG2	0.0	1.58
THR-18	THR_CCG2	1.7	0.25
VAL-21	VAL_NCG1	0.7	0.50
VAL-21	VAL_NCG2	1.1	0.94
VAL-21	VAL_CCG2	1.1	1.25
VAL-21	VAL_CCG1	2.5	3.37
THR-25	THR_NCG2	1.7	1.57
THR-25	THR_CCG2	2.6	0.25
VAL-39	VAL_NCG2	0.6	0.97
VAL-39	VAL_CCG1	0.9	0.61
VAL-39	VAL_NCG1	1.9	2.06
VAL-39	VAL_CCG2	3.3	4.04
VAL-42	VAL_NCG2	0.7	0.73
VAL-42	VAL_CCG1	1.3	0.95
VAL-42	VAL_NCG1	1.7	2.01
VAL-42	VAL_CCG2	3.0	4.05
THR-44	THR_NCG2	0.5	1.52
THR-44	THR_CCG2	2.9	0.81
THR-49	THR_NCG2	0.8	1.37
THR-49	THR_CCG2	3.0	1.22
THR-51	THR_CCG2	0.5	0.22
THR-51	THR_NCG2	1.6	1.57
THR-53	THR_CCG2	0.4	0.22
THR-53	THR_NCG2	1.6	1.56
VAL-54	VAL_CCG1	0.7	0.79

VAL-54	VAL_NCG1	0.9	0.93
VAL-54	VAL_CCG2	1.0	1.72
VAL-54	VAL_NCG2	1.8	1.51
THR-55	THR_CCG2	0.0	0.24
THR-55	THR_NCG2	1.5	1.51

Table S6. HA-CA-CB-HB *J*-Coupling data (Hz) for ubiqutin.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
MET-1	1_HA_1_CA_1_CB_1_1HB	4.3	3.54
ILE-3	3_HA_3_CA_3_CB_3_HB	4.7	4.80
PHE-4	4_HA_4_CA_4_CB_4_1HB	11.9	10.33
PHE-5	4_HA_4_CA_4_CB_4_2HB	3.6	4.04
VAL-5	5_HA_5_CA_5_CB_5_HB	9.6	10.47
LYS-6	6_HA_6_CA_6_CB_6_1HB	6.2	4.75
LYS-6	6_HA_6_CA_6_CB_6_2HB	7.0	8.69
LEU-8	8_HA_8_CA_8_CB_8_1HB	8.7	10.02
LEU-8	8_HA_8_CA_8_CB_8_2HB	4.1	3.31
LYS-11	11_HA_11_CA_11_CB_11_1HB	5.7	2.90
LYS-11	11_HA_11_CA_11_CB_11_2HB	6.7	10.52
ILE-13	13_HA_13_CA_13_CB_13_HB	7.7	10.31
LEU-15	15_HA_15_CA_15_CB_15_1HB	8.4	8.32
LEU-15	15_HA_15_CA_15_CB_15_2HB	1.4	4.92
GLU-16	16_HA_16_CA_16_CB_16_1HB	5.5	5.05
GLU-16	16_HA_16_CA_16_CB_16_2HB	8.2	6.41
VAL-17	17_HA_17_CA_17_CB_17_HB	2.7	8.78
GLU-18	18_HA_18_CA_18_CB_18_1HB	9.3	10.48
GLU-18	18_HA_18_CA_18_CB_18_2HB	2.5	2.57
PRO-19	19_HA_19_CA_19_CB_19_1HB	6.8	5.45
PRO-19	19_HA_19_CA_19_CB_19_2HB	7.3	9.66
SER-20	20_HA_20_CA_20_CB_20_1HB	9.4	9.61
SER-20	20_HA_20_CA_20_CB_20_2HB	3.0	3.39
ILE-23	23_HA_23_CA_23_CB_23_HB	10.2	10.45
ASN-25	25_HA_25_CA_25_CB_25_1HB	8.4	9.69
ASN-25	25_HA_25_CA_25_CB_25_2HB	5.3	4.66
VAL-26	26_HA_26_CA_26_CB_26_HB	9.9	10.60
LYS-27	27_HA_27_CA_27_CB_27_1HB	10.6	10.28
LYS-27	27_HA_27_CA_27_CB_27_2HB	2.4	3.18
LYS-29	29_HA_29_CA_29_CB_29_1HB	9.2	10.47
LYS-29	29_HA_29_CA_29_CB_29_2HB	1.9	3.49
ILE-30	30_HA_30_CA_30_CB_30_HB	10.5	10.57
GLN-31	31_HA_31_CA_31_CB_31_1HB	3.8	2.60
GLN-31	31_HA_31_CA_31_CB_31_2HB	11.3	10.44
ASP-32	32_HA_32_CA_32_CB_32_1HB	7.4	8.32
ASP-32	32_HA_32_CA_32_CB_32_2HB	5.3	5.66
LYS-33	33_HA_33_CA_33_CB_33_1HB	9.0	7.61
LYS-33	33_HA_33_CA_33_CB_33_2HB	4.0	4.04

GLU-34	34_HA_34_CA_34_CB_34_1HB	10.2	10.66
GLU-34	34_HA_34_CA_34_CB_34_2HB	4.4	3.01
ILE-36	36_HA_36_CA_36_CB_36_HB	8.8	10.52
PRO-37	37_HA_37_CA_37_CB_37_1HB	6.5	5.50
PRO-37	37_HA_37_CA_37_CB_37_2HB	7.0	8.57
PRO-38	38_HA_38_CA_38_CB_38_1HB	7.8	9.72
PRO-38	38_HA_38_CA_38_CB_38_2HB	5.4	5.19
ASP-39	39_HA_39_CA_39_CB_39_1HB	4.7	8.31
ASP-39	39_HA_39_CA_39_CB_39_2HB	4.4	5.13
GLN-40	40_HA_40_CA_40_CB_40_1HB	12.2	8.50
GLN-40	40_HA_40_CA_40_CB_40_2HB	2.0	4.64
ARG-42	42_HA_42_CA_42_CB_42_1HB	8.3	7.30
ARG-42	42_HA_42_CA_42_CB_42_2HB	4.3	5.26
LEU-43	43_HA_43_CA_43_CB_43_1HB	9.9	10.28
LEU-43	43_HA_43_CA_43_CB_43_2HB	1.5	2.86
ILE-44	44_HA_44_CA_44_CB_44_HB	8.0	10.24
PHE-45	45_HA_45_CA_45_CB_45_1HB	3.5	3.60
PHE-45	45_HA_45_CA_45_CB_45_2HB	9.8	10.54
LEU-50	50_HA_50_CA_50_CB_50_1HB	11.4	10.33
LEU-50	50_HA_50_CA_50_CB_50_2HB	3.9	3.88
GLU-51	51_HA_51_CA_51_CB_51_1HB	9.2	6.54
GLU-51	51_HA_51_CA_51_CB_51_2HB	3.2	6.59
ASP-52	52_HA_52_CA_52_CB_52_1HB	10	10.52
ASP-52	52_HA_52_CA_52_CB_52_2HB	1.3	3.33
ARG-54	54_HA_54_CA_54_CB_54_1HB	11.3	10.59
ARG-54	54_HA_54_CA_54_CB_54_2HB	1.4	2.92
THR-55	55_HA_55_CA_55_CB_55_HB	2.4	3.94
LEU-56	56_HA_56_CA_56_CB_56_1HB	9.9	10.32
LEU-56	56_HA_56_CA_56_CB_56_2HB	2.1	2.52
ASP-58	58_HA_58_CA_58_CB_58_1HB	11.4	10.53
ASP-58	58_HA_58_CA_58_CB_58_2HB	2.4	3.47
TYR-59	59_HA_59_CA_59_CB_59_1HB	10	10.62
TYR-59	59_HA_59_CA_59_CB_59_2HB	1.8	3.39
ASN-60	60_HA_60_CA_60_CB_60_1HB	6.7	8.02
ASN-60	60_HA_60_CA_60_CB_60_2HB	5.5	6.03
ILE-61	61_HA_61_CA_61_CB_61_HB	9.8	10.57
GLN-62	62_HA_62_CA_62_CB_62_1HB	11.1	10.10
GLN-62	62_HA_62_CA_62_CB_62_2HB	3.1	3.64
LYS-63	63_HA_63_CA_63_CB_63_1HB	3.5	4.06
LYS-63	63_HA_63_CA_63_CB_63_2HB	4.4	4.56
GLU-64	64_HA_64_CA_64_CB_64_1HB	9.9	10.06
GLU-64	64_HA_64_CA_64_CB_64_2HB	1.5	2.57
SER-65	65_HA_65_CA_65_CB_65_1HB	8.9	10.44

SER-65	65_HA_65_CA_65_CB_65_2HB	4.2	3.00
THR-66	66_HA_66_CA_66_CB_66_HB	10.6	10.61
HIE-68	68_HA_68_CA_68_CB_68_1HB	10.1	10.44
HIE-68	68_HA_68_CA_68_CB_68_2HB	2.0	3.00
LEU-69	69_HA_69_CA_69_CB_69_1HB	4.7	3.12
LEU-69	69_HA_69_CA_69_CB_69_2HB	9.5	10.26
VAL-70	70_HA_70_CA_70_CB_70_HB	7.3	10.37
ARG-72	72_HA_72_CA_72_CB_72_1HB	6.4	3.12
ARG-72	72_HA_72_CA_72_CB_72_2HB	6.6	10.01
LEU-73	73_HA_73_CA_73_CB_73_1HB	8.6	10.35
LEU-73	73_HA_73_CA_73_CB_73_2HB	4.5	3.02

Table S7. N/C-CA-CB-CG J-Coupling data (Hz) for ubiqutin.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
3_ILE	ILE_CCG2	3.7	4.06
3_ILE	ILE_NCG2	0.4	0.57
5_VAL	VAL_CCG1	0.0	0.57
5_VAL	VAL_CCG2	3.7	3.53
5_VAL	VAL_NCG1	1.8	2.04
5_VAL	VAL_NCG2	0.5	0.99
7_THR	THR_CCG2	2.7	0.58
7_THR	THR_NCG2	1.1	1.09
9_THR	THR_CCG2	3.0	1.28
9_THR	THR_NCG2	0.8	0.98
12_THR	THR_CCG2	0.4	0.21
12_THR	THR_NCG2	1.6	1.55
13_ILE	ILE_CCG2	1.7	0.42
13_ILE	ILE_NCG2	1.4	1.38
14_THR	THR_CCG2	0.8	2.46
14_THR	THR_NCG2	1.5	0.80
17_VAL	VAL_CCG1	3.9	3.36
17_VAL	VAL_CCG2	1.0	1.00
17_VAL	VAL_NCG1	0.2	1.72
17_VAL	VAL_NCG2	0.7	1.09
22_THR	THR_CCG2	3.4	3.34
22_THR	THR_NCG2	0.8	0.82
23_ILE	ILE_CCG2	0.9	0.46
23_ILE	ILE_NCG2	2.1	3.97
26_VAL	VAL_CCG1	0.8	0.79
26_VAL	VAL_CCG2	4.2	3.55
26_VAL	VAL_NCG1	2.2	2.09
26_VAL	VAL_NCG2	0.6	0.83
30_ILE	ILE_CCG2	1.0	1.06
30_ILE	ILE_NCG2	2.1	1.68
36_ILE	ILE_CCG2	0.7	3.96
36_ILE	ILE_NCG2	2.1	1.10
44_ILE	ILE_CCG2	0.8	0.45
44_ILE	ILE_NCG2	1.6	1.48
55_THR	THR_CCG2	3.0	3.20
55_THR	THR_NCG2	0.8	1.00
61_ILE	ILE_CCG2	1.0	0.55
61_ILE	ILE_NCG2	2.1	1.08

70_VAL	VAL_CCG2	2.4	0.83
70_VAL	VAL_NCG2	0.5	0.78

Table S8. C-CA-CB-CG *J*-Coupling data (Hz) for Ubiqutin.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
2_GLN	2_C_2_CA_2_CB_2_CG	2.4	0.80
3_ILE	3_C_3_CA_3_CB_3_CG1	1.0	2.23
3_ILE	3_C_3_CA_3_CB_3_CG2	3.8	1.85
4_PHE	4_C_4_CA_4_CB_4_CG	4.0	3.56
5_VAL	5_C_5_CA_5_CB_5_CG2	3.5	3.53
6_LYS	6_C_6_CA_6_CB_6_CG	2.0	1.89
7_THR	7_C_7_CA_7_CB_7_CG2	2.5	0.58
8_LEU	8_C_8_CA_8_CB_8_CG	2.6	2.63
9_THR	9_C_9_CA_9_CB_9_CG2	2.8	1.28
13_ILE	13_C_13_CA_13_CB_13_CG1	2.3	3.37
13_ILE	13_C_13_CA_13_CB_13_CG2	1.5	0.46
14_THR	14_C_14_CA_14_CB_14_CG2	0.7	2.90
15_LEU	15_C_15_CA_15_CB_15_CG	2.2	2.79
16_GLU	16_C_16_CA_16_CB_16_CG	1.8	1.32
17_VAL	17_C_17_CA_17_CB_17_CG1	3.6	3.28
17_VAL	17_C_17_CA_17_CB_17_CG2	0.9	0.73
19_PRO	19_C_19_CA_19_CB_19_CG	2.2	3.40
21_ASP	21_C_21_CA_21_CB_21_CG	5.5	4.19
22_THR	22_C_22_CA_22_CB_22_CG2	3.1	0.39
24_GLU	24_C_24_CA_24_CB_24_CG	1.5	0.90
25_ASN	25_C_25_CA_25_CB_25_CG	3.4	1.87
26_VAL	26_C_26_CA_26_CB_26_CG1	0.8	0.79
26_VAL	26_C_26_CA_26_CB_26_CG2	4.0	3.55
29_LYS	29_C_29_CA_29_CB_29_CG	4.0	3.58
31_GLN	31_C_31_CA_31_CB_31_CG	0.6	0.56
32_ASP	32_C_32_CA_32_CB_32_CG	3.3	3.93
33_LYS	33_C_33_CA_33_CB_33_CG	2.8	1.16
34_GLU	34_C_34_CA_34_CB_34_CG	2.9	3.57
38_PRO	38_C_38_CA_38_CB_38_CG	2.7	3.27
39_ASP	39_C_39_CA_39_CB_39_CG	1.8	3.56
40_GLN	40_C_40_CA_40_CB_40_CG	3.4	0.87
41_GLN	41_C_41_CA_41_CB_41_CG	3.5	3.53
42_ARG	42_C_42_CA_42_CB_42_CG	2.4	3.02
43_LEU	43_C_43_CA_43_CB_43_CG	3.0	3.27
44_ILE	44_C_44_CA_44_CB_44_CG1	3.1	3.35
44_ILE	44_C_44_CA_44_CB_44_CG2	0.7	0.45
48_LYS	48_C_48_CA_48_CB_48_CG	2.5	2.55

49_GLN	49_C_49_CA_49_CB_49_CG	1.4	0.72
50_LEU	50_C_50_CA_50_CB_50_CG	2.4	3.46
51_GLU	51_C_51_CA_51_CB_51_CG	2.9	1.91
54_ARG	54_C_54_CA_54_CB_54_CG	3.5	3.62
55_THR	55_C_55_CA_55_CB_55_CG2	2.8	0.50
56_LEU	56_C_56_CA_56_CB_56_CG	2.8	3.23
58_ASP	58_C_58_CA_58_CB_58_CG	5.6	4.18
59_TYR	59_C_59_CA_59_CB_59_CG	3.6	3.56
60_ASN	60_C_60_CA_60_CB_60_CG	2.0	4.22
61_ILE	61_C_61_CA_61_CB_61_CG1	3.3	2.98
61_ILE	61_C_61_CA_61_CB_61_CG2	0.8	0.57
63_LYS	63_C_63_CA_63_CB_63_CG	1.2	0.97
64_GLU	64_C_64_CA_64_CB_64_CG	3.4	0.66
66_THR	66_C_66_CA_66_CB_66_CG2	0.5	3.33
67_LEU	67_C_67_CA_67_CB_67_CG	3.4	3.28
68_HIE	68_C_68_CA_68_CB_68_CG	0.8	2.17
69_LEU	69_C_69_CA_69_CB_69_CG	0.8	0.74
72_ARG	72_C_72_CA_72_CB_72_CG	1.6	2.33
73_LEU	73_C_73_CA_73_CB_73_CG	2.8	3.53
74_ARG	74_C_74_CA_74_CB_74_CG	2.2	2.09

Table S9. HA-CA-CB-HB *J*-Coupling data (Hz) for hen egg white lysozyme.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
VAL-2	2_HA_2_CA_2_CB_2_HB	9.8	10.51
PHE-3	3_HA_3_CA_3_CB_3_1HB	7.7	9.61
PHE-3	3_HA_3_CA_3_CB_3_2HB	1.0	2.64
CYS-6	6_HA_6_CA_6_CB_6_1HB	12.6	10.55
CYS-6	6_HA_6_CA_6_CB_6_2HB	0.9	3.36
LEU-8	8_HA_8_CA_8_CB_8_1HB	1.2	4.10
MET-12	12_HA_12_CA_12_CB_12_1HB	12.6	10.52
MET-12	12_HA_12_CA_12_CB_12_2HB	1.0	2.63
HIE-15	15_HA_15_CA_15_CB_15_1HB	9.0	10.54
HIE-15	15_HA_15_CA_15_CB_15_2HB	0.6	3.48
LEU-17	17_HA_17_CA_17_CB_17_1HB	9.5	9.94
LEU-17	17_HA_17_CA_17_CB_17_2HB	1.0	2.45
ASP-18	18_HA_18_CA_18_CB_18_1HB	1.7	2.62
ASP-18	18_HA_18_CA_18_CB_18_2HB	13.2	10.45
TYR-20	20_HA_20_CA_20_CB_20_1HB	1.4	3.03
TYR-20	20_HA_20_CA_20_CB_20_2HB	12	10.67
TYR-23	23_HA_23_CA_23_CB_23_1HB	8.3	10.65
TYR-23	23_HA_23_CA_23_CB_23_2HB	0.2	3.30
SER-24	24_HA_24_CA_24_CB_24_1HB	1.0	3.31
ASN-27	27_HA_27_CA_27_CB_27_1HB	12.1	10.66
ASN-27	27_HA_27_CA_27_CB_27_2HB	0.5	3.20
CYS-30	30_HA_30_CA_30_CB_30_1HB	0.2	2.59
CYS-30	30_HA_30_CA_30_CB_30_2HB	6.8	10.51
LYS-33	33_HA_33_CA_33_CB_33_1HB	2.1	3.22
LYS-33	33_HA_33_CA_33_CB_33_2HB	7.9	10.52
PHE-34	34_HA_34_CA_34_CB_34_1HB	12.1	10.63
PHE-34	34_HA_34_CA_34_CB_34_2HB	1.6	3.13
PHE-38	38_HA_38_CA_38_CB_38_1HB	11.9	10.26
ASN-39	39_HA_39_CA_39_CB_39_1HB	2.2	5.00
ASN-39	39_HA_39_CA_39_CB_39_2HB	12.7	8.60
GLN-41	41_HA_41_CA_41_CB_41_1HB	10	9.16
GLN-41	41_HA_41_CA_41_CB_41_2HB	1.2	4.48
THR-43	43_HA_43_CA_43_CB_43_HB	3.9	10.07
THR-47	47_HA_47_CA_47_CB_47_HB	2.4	10.57
ASP-48	48_HA_48_CA_48_CB_48_1HB	0.2	3.92
ASP-48	48_HA_48_CA_48_CB_48_2HB	1.2	8.53

THR-51	51_HA_51_CA_51_CB_51_HB	13.3	10.53
ASP-52	52_HA_52_CA_52_CB_52_1HB	10.3	10.43
ASP-52	52_HA_52_CA_52_CB_52_2HB	0.3	3.56
TYR-53	53_HA_53_CA_53_CB_53_1HB	12.5	10.46
TYR-53	53_HA_53_CA_53_CB_53_2HB	0.8	3.50
ILE-55	55_HA_55_CA_55_CB_55_HB	3.6	2.93
ASN-59	59_HA_59_CA_59_CB_59_1HB	1.9	5.62
ASN-59	59_HA_59_CA_59_CB_59_2HB	8.1	4.66
CYS-64	64_HA_64_CA_64_CB_64_1HB	0.9	4.00
CYS-64	64_HA_64_CA_64_CB_64_2HB	0.5	3.45
ASN-65	65_HA_65_CA_65_CB_65_1HB	2.1	6.37
ASN-65	65_HA_65_CA_65_CB_65_2HB	13.4	6.41
ASP-66	66_HA_66_CA_66_CB_66_1HB	0.1	3.60
ASP-66	66_HA_66_CA_66_CB_66_2HB	2.2	3.92
THR-69	69_HA_69_CA_69_CB_69_HB	11.4	10.56
ASN-74	74_HA_74_CA_74_CB_74_1HB	1.7	4.49
ASN-74	74_HA_74_CA_74_CB_74_2HB	12.6	5.51
CYS-80	80_HA_80_CA_80_CB_80_1HB	13.8	10.25
CYS-80	80_HA_80_CA_80_CB_80_2HB	1.0	4.11
LEU-84	84_HA_84_CA_84_CB_84_1HB	12.0	10.13
LEU-84	84_HA_84_CA_84_CB_84_2HB	0.5	3.34
ASP-87	87_HA_87_CA_87_CB_87_2HB	12.2	9.88
ILE-88	88_HA_88_CA_88_CB_88_HB	2.0	3.63
THR-89	89_HA_89_CA_89_CB_89_HB	10.8	10.53
ASN-93	93_HA_93_CA_93_CB_93_1HB	13.5	10.56
ASN-93	93_HA_93_CA_93_CB_93_2HB	1.9	2.85
CYS-94	94_HA_94_CA_94_CB_94_1HB	2.1	3.04
CYS-94	94_HA_94_CA_94_CB_94_2HB	15.0	10.64
ILE-98	98_HA_98_CA_98_CB_98_HB	15.3	10.32
MET-105	105_HA_105_CA_105_CB_105_1HB	13.0	6.79
MET-105	105_HA_105_CA_105_CB_105_2HB	2.6	6.26
ASN-106	106_HA_106_CA_106_CB_106_1HB	13.2	10.59
ASN-106	106_HA_106_CA_106_CB_106_2HB	3.1	3.07
TRP-111	111_HA_111_CA_111_CB_111_1HB	1.7	3.20
ARG-114	114_HA_114_CA_114_CB_114_2HB	1.8	4.05
LYS-116	116_HA_116_CA_116_CB_116_1HB	3.4	3.08
LYS-116	116_HA_116_CA_116_CB_116_2HB	9.8	10.54
THR-118	118_HA_118_CA_118_CB_118_HB	4.9	3.14
ASP-119	119_HA_119_CA_119_CB_119_1HB	4.5	3.55
ASP-119	119_HA_119_CA_119_CB_119_2HB	13.3	10.48
VAL-120	120_HA_120_CA_120_CB_120_HB	4.5	3.50
TRP-123	123_HA_123_CA_123_CB_123_1HB	8.6	10.44
TRP-123	123_HA_123_CA_123_CB_123_2HB	0.3	3.07

ILE-124	124_HA_124_CA_124_CB_124_HB	4.2	10.06
CYS-127	127_HA_127_CA_127_CB_127_2HB	2.6	3.76

Table S9. C-CA-CB-HB *J*-Coupling data (Hz) for hen egg white lysozyme.

Residue index	Dihedral angel	*J*-expt.	*J*-calc.
2_VAL	2_C_2_CA_2_CB_2_HB	2.6	1.46
3_PHE	3_C_3_CA_3_CB_3_1HB	1.4	1.52
3_PHE	3_C_3_CA_3_CB_3_2HB	3.6	2.74
6_CYS	6_C_6_CA_6_CB_6_1HB	3.7	1.65
6_CYS	6_C_6_CA_6_CB_6_2HB	2.6	1.25
8_LEU	8_C_8_CA_8_CB_8_1HB	8.5	5.94
8_LEU	8_C_8_CA_8_CB_8_2HB	3.1	1.79
12_MET	12_C_12_CA_12_CB_12_1HB	1.8	1.37
12_MET	12_C_12_CA_12_CB_12_2HB	2.2	2.45
15_HIE	15_C_15_CA_15_CB_15_1HB	2.2	1.94
17_LEU	17_C_17_CA_17_CB_17_1HB	1.8	1.44
17_LEU	17_C_17_CA_17_CB_17_2HB	2.2	3.00
18_ASP	18_C_18_CA_18_CB_18_1HB	8.3	6.66
20_TYR	20_C_20_CA_20_CB_20_1HB	8.1	6.88
20_TYR	20_C_20_CA_20_CB_20_2HB	4.4	1.74
23_TYR	23_C_23_CA_23_CB_23_1HB	3.0	1.77
23_TYR	23_C_23_CA_23_CB_23_2HB	2.6	1.69
24_SER	24_C_24_CA_24_CB_24_1HB	1.3	1.41
24_SER	24_C_24_CA_24_CB_24_2HB	7.4	1.13
27_ASN	27_C_27_CA_27_CB_27_1HB	0.3	1.57
27_ASN	27_C_27_CA_27_CB_27_2HB	1.1	1.97
30_CYS	30_C_30_CA_30_CB_30_1HB	7.7	6.48
30_CYS	30_C_30_CA_30_CB_30_2HB	2.3	1.43
33_LYS	33_C_33_CA_33_CB_33_1HB	1.1	1.51
33_LYS	33_C_33_CA_33_CB_33_2HB	12.5	6.85
34_PHE	34_C_34_CA_34_CB_34_1HB	1.1	1.44
34_PHE	34_C_34_CA_34_CB_34_2HB	2.2	2.15
38_PHE	38_C_38_CA_38_CB_38_1HB	0.7	1.69
38_PHE	38_C_38_CA_38_CB_38_2HB	3.0	1.90
39_ASN	39_C_39_CA_39_CB_39_1HB	8.1	3.04
39_ASN	39_C_39_CA_39_CB_39_2HB	2.2	1.92
40_THR	40_C_40_CA_40_CB_40_HB	0.4	1.14
41_GLN	41_C_41_CA_41_CB_41_1HB	1.9	1.80
43_THR	43_C_43_CA_43_CB_43_HB	1.8	0.96
47_THR	47_C_47_CA_47_CB_47_HB	1.7	0.78
48_ASP	48_C_48_CA_48_CB_48_1HB	0.7	1.87
48_ASP	48_C_48_CA_48_CB_48_2HB	9.6	3.03
51_THR	51_C_51_CA_51_CB_51_HB	1.7	1.08

52_ASP	52_C_52_CA_52_CB_52_2HB	1.1	1.71
53_TYR	53_C_53_CA_53_CB_53_1HB	2.6	1.74
53_TYR	53_C_53_CA_53_CB_53_2HB	1.9	1.86
55_ILE	55_C_55_CA_55_CB_55_HB	7.0	6.58
59_ASN	59_C_59_CA_59_CB_59_1HB	8.5	4.77
64_CYS	64_C_64_CA_64_CB_64_1HB	2.1	1.22
64_CYS	64_C_64_CA_64_CB_64_2HB	8.0	6.56
65_ASN	65_C_65_CA_65_CB_65_1HB	8.1	4.07
65_ASN	65_C_65_CA_65_CB_65_2HB	1.0	2.72
66_ASP	66_C_66_CA_66_CB_66_1HB	1.4	1.88
66_ASP	66_C_66_CA_66_CB_66_2HB	10.9	6.67
74_ASN	74_C_74_CA_74_CB_74_1HB	6.6	4.85
74_ASN	74_C_74_CA_74_CB_74_2HB	0.1	3.35
80_CYS	80_C_80_CA_80_CB_80_1HB	2.8	1.57
80_CYS	80_C_80_CA_80_CB_80_2HB	0.9	1.30
84_LEU	84_C_84_CA_84_CB_84_1HB	2.6	2.24
84_LEU	84_C_84_CA_84_CB_84_2HB	1.5	1.74
89_THR	89_C_89_CA_89_CB_89_HB	3.3	0.78
92_VAL	92_C_92_CA_92_CB_92_HB	1.3	1.58
94_CYS	94_C_94_CA_94_CB_94_1HB	9.8	6.56
94_CYS	94_C_94_CA_94_CB_94_2HB	3.1	1.19
98_ILE	98_C_98_CA_98_CB_98_HB	1.8	1.12
105_MET	105_C_105_CA_105_CB_105_1HB	1.1	2.14
105_MET	105_C_105_CA_105_CB_105_2HB	1.4	4.20
106_ASN	106_C_106_CA_106_CB_106_1HB	3.0	1.50
106_ASN	106_C_106_CA_106_CB_106_2HB	3.0	2.15
116_LYS	116_C_116_CA_116_CB_116_1HB	8.5	6.81
116_LYS	116_C_116_CA_116_CB_116_2HB	2.2	1.72
118_THR	118_C_118_CA_118_CB_118_HB	1.8	1.16
120_VAL	120_C_120_CA_120_CB_120_HB	3.0	1.64
123_TRP	123_C_123_CA_123_CB_123_1HB	1.1	1.50
123_TRP	123_C_123_CA_123_CB_123_2HB	1.8	2.23
124_ILE	124_C_124_CA_124_CB_124_HB	0.8	1.47
127_CYS	127_C_127_CA_127_CB_127_2HB	0.8	1.28