

residue X	XA Ca shift			XP Ca Shift				
	Calc		Expt	Diff	Calc	Expt	Diff	
Ala	52.5	69	52.5	0.0	50.5	78	50.5	0.0
Cys (red)	57.0	10	58.2	-1.2	55.7	10	56.4	-0.7
Asp	54.0	82	54.2	-0.2	51.6	46	52.2	-0.6
Glu	56.3	55	56.6	-0.3	54.0	39	54.2	-0.2
Phe	57.2	27	57.7	-0.5	55.5	33	55.6	-0.1
Gly	45.1	93	45.1	0.0	44.1	65	44.5	-0.4
His	55.5	16	55.0	0.5	54.0	25	53.3	0.7
Ile	61.2	31	61.1	0.1	57.8	58	58.7	-0.9
Lys	56.6	58	56.2	0.4	54.0	68	54.2	-0.2
Leu	54.9	44	55.1	-0.2	52.5	104	53.1	-0.6
Met	55.8	17	55.4	0.4	53.2	21	53.3	-0.1
Asn	52.8	46	53.1	-0.3	51.2	71	51.3	-0.1
Pro	63.0	59	63.3	-0.3	61.2	43	61.5	-0.3
Gln	56.3	33	55.7	0.6	53.4	40	53.7	-0.3
Arg	55.5	29	56.0	-0.5	54.1	48	54.0	0.1
Ser	58.5	68	58.3	0.2	56.1	69	56.4	-0.3
Thr	61.7	41	61.8	-0.1	58.9	60	59.8	-0.9
Val	61.9	35	62.2	-0.3	59.5	72	59.8	-0.3
Trp	55.9	4	57.5	-1.6	60.7	1	55.7	5.0
Tyr	56.6	11	57.9	-1.3	54.9	33	55.8	-0.9

Database-derived values are listed under 'Calc'; 'Expt' are experimentally derived values of Schwarzingler et al (2000). Number of shifts contributing to the calculated average are shown to the right of the value.