

Appendix A

Side Chain Chemical Shift Lists

The chemical shift lists for the protein disulphide isomerase N-terminal thioredoxin-like domain spin system results are given in this appendix. Chemical shift values in **bold** are ones which have been correctly identified by the program; chemical shift values in plain text are erroneous. The “Assign” column of these tables shows the position of the result in the sequence, if appropriate. If the result is a composite of more than one spin system, the word “Mix” appears in this column; the word “Partial” after an assignment indicates that part of a spin system has been found. If a misassignment has taken place, then a star will appear in this column, followed by the residue to which the peaks actually belong. No entry at all means that something is visible in the spectra, but this does not correspond to a known spin system. The “Resp” and “Orig” columns show the score of the result before and after penalisation algorithms have been applied, respectively.

Glycine results set:

Resl	H α'	H α	C α	Resp	Orig	Assign
0	3.68	3.29	44.5	3097	5560	G81 Partial
1	3.69	4.24	45.1	3771	4422	G117 Partial
2	3.88	4.05	44.2	5802	7028	G57 Partial
3	3.97	3.49	46.7	6270	16568	G51
4	3.66	3.50	43.6	8034	20949	G81
5	3.74	3.85	46.7	10975	12630	G78
6	3.93	4.21	47.9	13994	17491	G37
7	3.90	4.11	45.4	17018	17769	G57
8	3.88	3.50	45.8	19021	19021	G91
9	4.27	4.08	44.5	85883	86244	G117

Alanine results set:

Resl	H β_3	H α	C α	C β	Resp	Orig	Assign
0	0.90	4.08	53.6	20.4	1356	5910	Mix
1	0.58	4.13	57.3	24.2	2118	11803	L73
2	1.52	4.11	57.6	24.5	2226	11340	Mix
3	1.43	4.29	55.8	18.9	2696	10900	Mix

4	1.21	4.36	52.0	17.9	3000	11618	
5	1.57	4.41	54.8	17.3	3386	16301	Mix
6	1.60	3.66	49.2	17.6	3538	4090	A74 Partial
7	1.40	4.82	50.1	17.3	3687	5010	Water
8	1.55	3.74	56.7	17.3	3870	18120	
9	1.57	4.38	50.8	17.3	4016	14303	
10	1.82	3.41	49.5	23.9	4141	4228	P83
11	1.43	4.11	50.1	15.1	4165	5993	A43 Partial
12	1.60	4.02	57.6	17.6	4372	23406	A47
13	1.41	4.21	57.0	18.3	5832	18040	A43 Partial
14	1.33	3.80	52.6	17.6	5951	6898	A49 Partial
15	1.88	3.61	49.8	24.2	6316	8420	P3
16	1.32	4.10	55.1	21.4	6647	20737	A20 Partial
17	1.54	4.16	57.0	17.3	13683	85678	L73
18	1.36	4.43	49.8	22.0	13808	16215	Mix
19	1.36	4.58	52.0	17.0	13863	16818	Mix
20	1.46	4.14	52.0	15.1	21647	36975	A43 Partial
21	1.46	4.18	57.0	15.1	26191	109797	A43
22	1.32	4.14	55.1	19.8	38806	133807	A20 Partial
23	1.36	3.75	54.8	17.6	40806	113029	A49
24	1.29	4.14	54.8	18.3	41614	115005	A20
25	1.58	3.71	54.8	17.9	42686	126080	A74
26	1.21	4.44	50.4	17.9	44553	112341	A101
27	1.36	4.02	52.9	17.9	50687	142698	A22
28	1.40	4.25	52.6	18.6	58613	72795	
29	-0.35	4.30	48.3	19.8	61128	68306	A33
30	1.55	4.11	51.4	17.3	65852	84236	
31	1.46	3.91	54.8	20.4	69114	91289	A18
32	1.30	4.11	53.9	18.3	88173	176346	A120 Partial
33	1.29	5.74	49.5	25.4	108409	109429	A63
34	1.38	4.60	50.1	17.6	110735	332205	A2
35	1.46	3.88	52.9	20.4	121912	125133	A67
36	1.50	3.90	56.4	18.9	127336	134547	A105
37	0.99	4.05	52.3	18.9	135596	144797	A23
38	1.55	4.25	53.9	17.9	147920	162392	A41
39	1.61	4.60	52.9	19.5	156734	164066	A94
40	1.33	4.10	53.6	19.8	162361	575499	A120
41	1.50	3.93	54.8	18.9	165410	183933	A50
42	1.40	4.38	52.0	18.6	167334	576744	A119

AMX results set:

Resl	$H\beta$	$H\alpha$	$C\alpha$	$C\beta$	$H\beta'$	Resp	Orig	Assign
0	1.29	5.74	49.5	25.4	1.29	113	21877	*A63
1	2.63	4.85	56.4	40.8	2.63	124	1626	F88 Partial
2	2.77	4.66	54.5	38.3	2.77	126	4338	D1 Partial
3	2.04	5.02	54.5	40.4	2.04	130	852	*K40
4	1.79	5.18	52.9	32.9	1.68	140	42801	*R89
5	2.05	3.68	49.5	26.7	2.05	148	28591	*K40
6	2.44	4.88	52.6	29.8	2.44	149	720	
7	1.71	3.75	56.1	42.3	1.71	149	2884	*L42
8	3.04	4.27	56.1	33.6	4.22	162	1635	
9	1.35	5.44	49.2	43.9	1.35	173	418	*R61
10	3.08	4.82	55.8	45.1	3.08	184	2503	*S95

11	2.00	3.86	50.1	27.3	2.00	184	7096	*Q76
12	1.71	4.10	59.2	31.7	1.71	196	3371	*K54
13	1.54	3.68	54.8	41.4	1.54	200	1935	*L21
14	1.55	4.11	51.7	42.6	1.55	205	3951	*L73
15	2.19	4.74	53.9	45.1	2.19	206	1341	*K97
16	2.18	3.97	50.1	31.4	2.18	222	2138	*K14
17	3.21	4.27	57.0	39.5	3.21	242	5841	
18	1.80	4.83	52.3	26.7	1.80	243	2816	*E70
19	2.75	4.43	57.3	37.3	2.75	247	2534	
20	2.65	4.21	55.1	32.3	2.65	270	1304	
21	1.38	4.88	50.1	32.3	1.38	334	805	*R61
22	1.63	4.57	52.6	34.5	1.63	345	9278	*R13
23	1.82	3.41	49.5	23.9	1.82	351	845	*K113
24	2.96	4.64	57.9	25.4	2.96	381	918	
25	1.49	4.99	54.8	43.3	1.49	385	1856	*L62
26	3.13	4.58	57.6	28.9	3.13	395	952	H38 Partial
27	2.10	3.97	60.8	28.6	2.10	398	5181	*E19
28	3.94	4.89	55.4	42.3	3.94	430	1036	*S95
29	1.65	4.21	56.1	30.4	1.65	443	4512	*R115
30	1.86	3.57	49.8	26.7	1.86	447	1077	*K52
31	1.60	3.99	57.6	41.1	1.74	522	19654	*L53
32	2.15	4.43	55.8	29.8	1.71	536	54348	*R103
33	4.11	4.79	63.6	39.8	4.11	548	1321	*T84
34	2.25	4.11	61.4	29.5	2.25	553	1331	*E45
35	2.11	3.25	51.1	27.3	2.11	570	2744	*E56
36	2.18	3.63	57.6	42.3	1.27	591	22256	*L112
37	1.38	5.27	53.6	37.6	1.38	592	3854	*K86
38	1.58	4.36	50.8	42.3	1.58	605	2914	*L10
39	2.36	4.19	54.5	26.7	2.36	715	9311	*A41
40	3.40	4.52	58.6	28.6	3.40	769	1852	*Q75
41	3.22	4.18	57.6	26.4	3.55	773	18621	H8 Partial
42	1.60	4.22	52.0	42.9	1.60	800	1927	*L10
43	3.18	4.83	53.9	34.5	3.02	802	13654	H24 Partial
44	1.97	3.61	50.1	24.2	1.90	846	2038	*K48
45	1.85	4.14	60.8	42.3	1.85	873	2102	*K52
46	2.93	4.88	53.9	29.5	3.04	905	19178	H24
47	3.11	4.22	57.0	38.3	3.22	1045	25157	
48	1.90	4.08	59.5	32.0	2.04	1099	112383	*K40
49	2.94	4.82	56.7	45.1	2.58	1980	15083	F88
50	2.21	4.13	58.6	29.5	2.21	2077	5000	E45
51	2.58	4.36	57.3	39.8	2.58	2080	20026	D106
52	4.21	4.27	63.3	33.6	3.05	2218	3169	C39
53	2.75	4.80	53.9	40.8	3.22	2323	30049	D92
54	3.21	4.69	58.3	29.8	3.21	2332	5613	H38
55	3.88	4.91	55.4	44.2	3.88	2402	5782	
56	2.21	4.58	55.1	31.1	1.99	2863	44743	*E59
57	2.86	5.18	53.6	40.1	3.02	2935	23869	Y82
58	3.18	4.91	56.1	37.9	2.85	3155	9468	
59	3.16	5.22	54.8	41.7	3.05	3196	29604	Y26
60	3.65	4.68	53.9	27.9	3.27	3296	32962	W35
61	2.80	4.43	56.1	37.9	3.05	4117	139092	N110
62	2.15	4.43	56.7	31.1	1.99	4281	32997	*E69
63	2.57	4.46	55.8	41.7	2.80	5051	15160	Y32
64	2.33	4.44	63.3	31.7	2.02	5755	303803	*P3
65	1.32	5.44	53.6	44.2	2.35	6287	21358	*L28

66	2.40	4.61	62.3	34.2	2.21	6506	24469	
67	3.18	4.46	58.9	40.1	2.99	6867	20608	
68	2.58	5.04	54.8	42.0	2.77	7177	21593	Y32
69	3.65	4.08	62.0	30.1	3.49	11264	27110	W111
70	2.96	4.61	57.6	38.6	3.07	11265	27114	
71	3.27	4.58	58.6	37.3	2.15	12551	43154	Y77
72	2.52	5.35	62.9	33.9	1.85	13456	21025	*P83
73	3.30	4.02	58.6	38.9	3.15	17918	43125	
74	3.15	3.79	62.3	38.9	2.68	19662	47321	Y46
75	2.72	4.47	57.0	39.8	2.61	20730	169053	D72
76	3.11	3.91	63.3	39.8	3.27	22266	53589	F17
77	2.21	4.11	57.9	32.3	1.77	24678	92573	Mix
78	3.27	5.71	55.1	42.0	3.40	29049	29049	F87
79	2.83	5.57	57.0	40.1	3.49	39413	39413	F31
80	3.02	4.27	54.2	37.3	2.88	41714	112742	N90
81	1.90	3.91	57.9	38.6	2.68	42210	42210	Y99
82	2.29	3.30	52.0	38.3	2.90	45975	45975	D66
83	2.77	5.24	52.0	39.2	3.36	73359	73359	N16
84	2.52	3.99	55.1	39.8	2.86	82277	82277	D7
85	2.74	4.69	54.2	41.1	2.58	119914	405116	D1

Serine results set:

Resl	H β	H α	C α	C β	H β'	Resp	Orig	Assign
0	3.71	4.83	54.5	57.9	3.71	50	489	*C36
1	2.99	4.58	57.6	59.8	2.99	105	931	*D107
2	4.02	3.72	50.1	63.6	4.02	120	1608	
3	3.05	4.88	53.9	55.1	3.05	161	568	*H24
4	3.02	4.25	56.1	59.2	3.02	229	975	*C39
5	3.94	4.21	47.9	62.6	4.16	366	2820	*S71
6	4.22	3.93	47.9	61.4	4.22	417	5770	*E19
7	4.58	4.79	50.1	65.8	4.58	459	666	*D92
8	4.27	4.43	54.2	69.5	4.27	721	1130	*T93
9	4.44	3.66	50.1	62.9	4.46	791	16960	*G81
10	3.15	4.82	53.9	57.3	3.16	1182	2071	*D92
11	3.96	4.25	61.1	62.6	4.22	8163	13306	S71 Partial
12	3.88	4.46	58.3	63.6	3.91	9700	10286	
13	3.93	4.94	55.4	62.9	3.96	13431	15793	S95
14	3.69	4.32	58.3	63.9	4.00	16436	38026	S58
15	3.93	4.30	59.8	62.6	4.04	26442	82206	S15

Threonine results set:

Resl	H β	H α	C α	C β	H γ_{23}	C γ	Resp	Orig	Assign
0	4.05	4.08	58.3	62.6	1.32	21.4	110	590	T84
1	3.41	3.41	67.0	68.3	0.35	20.4	112	223	*V109
2	3.69	3.69	57.3	63.9	1.18	16.7	113	142	*L21
3	4.07	4.07	62.6	63.9	0.66	19.2	134	251	*W111
4	3.88	3.91	56.4	63.9	1.47	17.3	140	327	*S95
5	4.21	4.21	55.8	62.9	0.88	17.9	143	621	*I60
6	3.61	3.61	57.0	63.6	0.18	16.7	160	318	*L112
7	3.77	3.75	57.0	62.6	1.15	17.6	163	531	*L21
8	3.72	3.71	55.4	63.6	1.38	22.0	164	358	*S95

9	4.16	4.18	55.4	69.8	1.19	20.8	173	469	
10	4.13	4.11	62.3	72.3	0.69	17.6	187	225	
11	4.30	4.25	61.4	63.6	0.33	17.6	193	833	*S71
12	4.16	4.14	60.8	72.0	0.91	20.1	208	250	*I60
13	4.10	4.08	62.6	64.5	1.33	21.4	237	237	T84 Partial
14	4.10	4.10	62.3	64.2	0.93	20.4	240	288	*W111
15	4.21	4.19	57.0	62.6	0.50	21.1	262	1129	*A43
16	3.94	3.91	55.4	69.8	0.57	20.1	264	1692	T116 Partial
17	4.36	4.36	57.6	65.1	1.40	20.4	268	699	*D106
18	4.33	4.32	58.3	64.8	0.30	16.1	351	525	*S58
19	4.38	4.38	55.1	65.1	1.49	16.7	361	1290	*R80
20	4.21	4.21	56.7	62.6	0.88	23.3	367	1194	*S71
21	4.29	4.29	58.3	70.1	0.66	21.1	377	452	
22	4.32	4.30	59.5	62.9	0.88	16.1	428	643	*S15
23	4.25	4.25	61.1	62.9	0.52	18.9	442	1151	
24	3.90	3.91	54.8	62.9	0.46	21.7	475	1547	*A50
25	3.85	3.85	61.4	64.8	0.50	16.7	597	892	
26	4.33	4.35	65.1	68.3	0.57	18.6	642	770	
27	4.30	4.30	60.1	67.9	0.47	20.4	688	1497	T68 Partial
28	3.69	4.30	57.9	63.9	0.38	19.2	689	16086	*S58
29	4.72	4.75	56.1	69.5	1.38	21.7	716	858	T93 Partial
30	3.93	3.93	54.8	62.6	1.27	18.6	815	1772	*S71
31	4.27	4.30	58.3	62.9	1.21	20.4	1371	1371	
32	4.27	4.29	63.3	69.8	1.21	22.9	2270	2270	T68 Partial
33	4.32	4.29	63.3	68.3	1.22	20.8	2747	2747	T68 Partial
34	4.52	4.47	60.4	68.9	1.10	20.8	2893	2893	T100
35	3.94	4.30	59.8	62.6	1.25	22.6	7760	42581	*S15
36	4.05	4.32	59.8	62.9	0.63	18.9	11699	33045	*S15
37	3.94	4.94	55.8	62.9	0.10	17.9	18903	58489	*S95
38	3.94	4.27	61.4	62.6	0.13	17.9	27888	82024	*S71
39	3.96	4.27	61.1	69.5	0.55	20.4	102228	190724	T116

Valine results set:

Resl	H β	H α	C α	C β	H γ_3	C γ_3	H γ'_3	C γ'_3	Resp	Orig	Assign
0	2.29	4.08	61.1	32.3	0.88	20.4	0.91	21.4	7940	15881	V9
1	1.90	4.25	62.6	31.4	0.91	19.8	0.88	20.8	10195	14981	V11
2	2.18	4.36	61.4	34.5	0.79	21.4	0.25	22.3	94778	120110	V29
3	1.30	4.32	60.1	36.4	0.49	21.4	0.71	20.4	123100	138403	V65
4	1.75	3.58	63.9	30.4	0.79	21.4	0.16	20.4	124827	177957	V79
5	2.11	3.41	67.6	31.4	0.91	21.4	1.05	22.9	141060	212059	V109

Isoleucine results set:

Resl	H β	H α	C α	C β	H γ 23	C γ 2	H γ 1	C γ 1	H γ 1'	H δ 3	C δ	Resp	Assign
0	1.86	4.14	61.1	37.9	0.91	16.7	1.19	27.0	1.47	0.86	12.3	4611	
1	1.82	4.18	62.9	38.3	0.88	17.9	0.93	27.9	1.77	0.80	13.9	12007	I60
2	1.77	3.85	64.8	38.6	0.47	16.4	0.58	27.3	1.85	0.63	12.9	39044	I108
3	1.99	5.55	60.1	38.9	0.72	17.9	0.66	27.6	1.61	0.77	12.9	95047	I85

Leucine results set:

Resl	H β	H α	C α	H β'	H δ_3	H γ	C γ	C δ_3	H δ'_3	C δ'_3	Resp	Assignment
0	1.29	4.32	60.1	1.32	0.47	0.68	22.3	21.1	0.71	20.8	157	*V65
1	1.74	3.99	57.6	1.60	0.66	1.71	27.0	26.1	0.88	22.0	161	L53
2	1.65	4.39	55.4	1.68	0.69	1.47	27.0	26.1	0.96	24.2	2422	L42
3	1.38	5.25	52.3	1.71	0.44	1.49	26.7	26.7	0.68	22.6	2564	L12
4	1.66	4.38	55.4	1.29	0.58	1.71	26.7	25.1	0.80	22.9	3322	L10
5	1.50	5.00	54.8	1.16	0.50	1.52	30.4	23.6	-0.06	25.4	3809	L62
6	2.18	3.63	57.6	1.25	0.83	2.15	26.4	27.3	0.72	23.9	4572	L112
7	2.35	5.44	53.6	1.32	0.63	1.72	26.4	26.1	0.97	23.9	6808	L28
8	1.16	5.43	53.3	1.80	0.29	1.18	26.7	25.8	0.55	23.9	13599	LL27
9	1.54	4.14	57.3	1.80	0.60	1.65	26.7	23.9	0.49	22.9	33381	L73
10	1.18	3.69	56.7	1.50	0.32	0.99	26.4	25.1	0.07	23.3	183810	L21