Appendix B

Backbone Chemical Shift Lists

The chemical shift lists for the protein disulphide isomerase N-terminal thioredoxin-like domain backbone results are given in this appendix. The symbols used are essentially the same as for the spin system results (see Appendix A). There is one difference: assignments are simply given a number, indicating their position in the sequence, if they are correct. If they are *not* correct, then the single letter code for the best fitting residue is placed in in the "Assign" column. A "G prev" in the assignment column means that the predecessor to the current residue is a glycine, which is not detected by the XX pattern.

Results set for non-glycine pairs:

Resl	H#1	N#1	CO	CO#1	Cα#1	Cα	Cβ#1	Cβ	Resp	Orig	Assign
0	**8.43**	**128.3**	——	——	55.6	**63.2**	42.4	55.0	8605	24217	12
1	**7.11**	**118.8**	——	——	**60.7**	**58.8**	**70.2**	**39.2**	9553	40140	100
2	8.19	127.7	——	——	**53.1**	62.0	**19.0**	70.8	12682	52724	
3	**8.03**	118.2	——	——	62.0	**58.8**	70.8	39.2	13092	53879	
4	**8.78**	**119.1**	——	——	64.5	**63.8**	**72.7**	**34.2**	20540	81138	84
5	**8.93**	**128.3**	——	——	**52.5**	**60.7**	**38.6**	**36.7**	22831	59419	66
6	**6.27**	**118.5**	——	——	**48.7**	**55.6**	**20.3**	**42.4**	24712	64383	33
7	**9.80**	**128.0**	——	——	**62.6**	**54.4**	**34.8**	**44.9**	25686	65846	29
8	**8.37**	122.8	——	——	56.9	**63.8**	33.5	**32.9**	26400	68628	
9	8.15	115.4	——	——	62.6	**55.0**	**53.7**	41.8	26523	67377	
10	**9.25**	**127.1**	——	——	**57.5**	**59.4**	**31.0**	**64.5**	27457	105676	59
11	**9.84**	**126.5**	——	——	**56.9**	**55.6**	**19.7**	**31.7**	28367	72045	105
12	8.29	133.3	——	——	55.0	**55.0**	**19.7**	43.0	28435	73099	
13	**8.76**	**125.6**	——	——	**63.2**	**58.8**	**39.2**	**30.4**	29014	74183	46
14	**8.14**	**125.3**	——	——	**60.1**	**64.5**	**32.3**	**34.2**	29490	76220	40
15	8.54	111.7	——	——	**57.5**	**57.5**	45.5	30.4	31941	81952	
16	**8.74**	**117.9**	——	——	**64.5**	**59.4**	**34.2**	**31.0**	33541	84724	39
17	8.42	109.8	——	——	46.8	**53.1**	45.5	**19.0**	35366	90042	
18	**8.78**	**131.1**	——	——	**53.7**	**52.5**	**20.9**	**38.6**	36834	92038	67
19	**8.86**	**126.2**	——	——	**55.0**	55.6	**41.8**	32.9	36868	92137	1
20	**9.50**	**121.9**	——	——	**50.0**	**55.0**	**26.0**	**43.6**	39269	97839	63
21	**8.62**	**124.0**	——	——	**63.8**	**57.5**	**38.6**	**31.0**	41415	103767	60
22	**9.18**	**132.7**	——	——	**54.4**	**54.4**	**44.9**	**46.8**	44937	111426	28
23	**8.86**	**129.9**	——	——	**55.6**	**64.5**	**31.7**	**31.0**	49016	119375	80

24	7.26	116.9	——	——	55.0	53.1	30.4	19.0	58113	138454	24
25	9.82	132.3	172.7	174.7	60.7	64.5	39.9	72.7	64743	125855	85
26	8.10	118.5	178.1	177.8	65.7	65.7	32.3	39.2	102231	107022	109
27	8.53	127.1	176.4	176.3	63.2	63.2	19.0	34.8	107732	123390	
28	9.25	125.9	173.2	175.8	55.6	52.5	43.6	32.3	116676	124838	62
29	8.34	124.6	172.2	178.3	60.1	55.0	52.5	30.4	118183	126868	25
30	7.46	118.8	179.1	178.1	58.8	60.7	32.3	53.7	123579	137738	114
31	9.74	124.9	173.8	173.5	56.3	54.4	42.4	38.6	129173	157976	87
32	9.40	126.8	174.7	173.8	54.4	60.7	38.6	39.9	132435	142155	86
33	7.20	117.6	177.7	179.1	53.7	57.5	18.4	42.4	143988	150035	22
34	9.40	130.5	173.5	173.9	57.5	55.6	41.8	42.4	146274	163026	88
35	7.08	119.7	180.6	177.7	58.8	66.4	30.4	31.0	157069	173426	45
36	7.52	122.5	178.6	178.1	65.7	57.5	39.2	41.1	185736	271141	108
37	7.35	120.6	182.8	178.6	58.2	58.2	41.1	41.1	194921	204572	107
38	7.43	118.8	179.1	178.1	58.2	60.7	56.9	31.7	198028	233222	114
39	9.08	126.5	176.4	175.6	56.9	55.0	31.0	34.8	199412	253019	98
40	8.37	117.9	177.2	175.2	63.8	54.4	70.2	41.1	200218	406223	93
41	9.12	129.3	175.9	175.8	56.3	62.0	43.6	32.9	207811	254292	10
42	8.39	119.7	179.2	180.0	58.2	62.6	43.0	30.4	211763	257968	112
43	8.35	121.6	177.3	175.8	55.6	57.5	33.5	31.0	220956	295113	5
44	9.96	124.3	176.7	176.6	55.0	53.7	38.0	33.5	234546	330988	90
45	6.92	123.4	175.8	177.3	57.5	63.8	31.7	68.9	239923	543642	69
46	8.66	108.6	181.5	176.1	48.7	55.6	47.4	19.0	242511	290281	G51
47	8.29	123.1	177.8	179.4	62.6	56.9	30.4	38.6	251932	318695	111
48	8.63	110.5	177.0	175.8	64.5	53.7	63.2	20.3	253246	488422	68
49	8.22	117.9	183.1	180.0	59.4	55.6	28.5	18.4	253668	272056	75
50	9.04	122.5	175.5	169.9	55.6	57.5	42.4	40.5	255781	361790	32
51	7.99	124.9	176.9	176.3	63.8	53.1	51.9	39.9	256295	374923	17
52	8.27	116.6	175.0	173.6	62.6	59.4	42.4	32.9	263196	411262	26
53	7.89	119.1	177.2	180.9	55.6	63.2	18.4	39.9	264047	288018	47
54	8.47	120.3	180.0	179.1	60.7	58.2	32.3	43.0	265415	337539	113
55	8.96	123.7	173.9	176.6	53.7	57.5	33.5	41.8	266203	403783	89
56	8.51	122.8	177.5	178.9	58.2	62.0	40.5	63.2	269578	512650	72
57	7.40	122.2	177.7	176.6	57.5	56.3	15.2	43.0	274509	324549	43
58	9.09	124.3	176.3	178.4	61.3	54.4	31.7	34.8	276869	321707	14
59	8.67	122.8	177.2	176.4	55.0	63.8	34.8	31.0	288152	347166	97
60	8.31	121.6	177.3	176.9	53.1	58.2	27.2	31.7	293059	470343	70
61	8.13	123.4	180.0	177.3	56.3	55.0	42.4	41.1	294932	509704	76
62	8.03	124.6	180.5	179.4	64.5	53.1	40.5	39.9	299325	495336	55
63	8.89	123.7	175.8	176.3	55.6	55.6	31.7	33.5	301393	441913	6
64	8.50	127.7	173.5	175.3	58.8	56.9	39.2	31.0	308410	459288	99
65	9.54	122.5	175.8	172.4	55.0	50.0	36.7	26.0	312303	511128	64
66	9.36	109.8	175.6	173.9	45.5	55.0	46.8	38.0	320815	605053	G91
67	7.47	119.7	179.1	177.3	53.7	53.7	19.0	18.4	329225	413948	23
68	7.55	117.2	176.9	177.5	53.1	53.1	27.2	27.2	345719	546748	71
69	8.02	124.0	175.0	173.3	55.6	59.4	17.8	32.3	346587	463386	55
70	7.42	117.9	179.2	176.4	56.9	58.2	31.0	18.4	347625	445397	115 Mix
71	8.01	122.5	180.9	180.0	60.1	55.0	32.9	18.4	363844	521864	48
72	7.95	120.9	178.3	181.5	64.5	55.6	19.0	47.4	366110	469399	50
73	8.33	124.9	172.2	178.3	53.7	60.1	20.3	32.9	396681	538397	49 Mix
74	7.54	121.2	178.7	179.2	55.0	60.1	18.4	32.3	397662	618172	41
75	7.97	120.3	178.0	179.4	55.6	58.2	18.4	43.6	405770	515512	74
76	8.71	124.0	176.9	175.5	57.5	63.2	30.4	32.3	407801	428804	4
77	7.94	113.9	178.6	172.2	56.3	53.7	55.0	20.3	420532	854628	95
78	8.23	120.3	181.2	178.7	60.1	55.6	29.1	17.8	430907	499378	19

79	**7.67**	**111.4**	**174.4**	**172.1**	46.2	**62.0**	**44.9**	**70.8**	440311	848437	G117
80	**7.85**	**124.9**	**178.7**	**179.7**	**55.6**	**60.1**	**19.0**	**29.1**	460729	756067	20
81	**7.54**	**115.4**	**179.4**	**177.0**	**56.9**	**55.0**	**30.4**	**17.8**	475581	726196	56
82	**9.00**	**119.4**	**174.4**	**176.3**	**54.4**	**53.7**	**34.8**	**44.3**	477934	659581	13
83	**7.62**	**119.1**	175.3	176.9	53.1	**55.6**	**42.4**	**19.0**	485949	740066	21
84	**8.88**	**120.6**	**176.3**	**181.2**	**55.6**	**63.8**	**17.8**	**40.5**	486312	639348	18
85	**7.89**	**113.6**	**175.**	**176.**	56.3	53.7	46.2	19.7	507601	879585	58 G prev
86	**7.86**	**122.5**	**178.9**	**178.0**	**58.2**	**58.2**	**43.6**	**40.5**	520259	782423	73
87	**7.60**	**109.8**	**174.9**	**175.0**	48.7	**59.4**	47.4	**38.0**	520760	862200	G78
88	**7.97**	**117.9**	**175.0**	**178.0**	**55.6**	**55.6**	**31.7**	**29.8**	535844	770223	104
89	**8.19**	**110.2**	**178.4**	**175.3**	**60.7**	**61.3**	59.4	**31.7**	545255	850729	15
90	**7.75**	**120.9**	173.9	**180.5**	**59.4**	**58.8**	**31.7**	**41.8**	553288	925835	54
91	**8.92**	**115.4**	**179.2**	**178.3**	**58.2**	**57.5**	**40.5**	**19.7**	556662	915514	106 G prev
92	**8.03**	*110.8*	**177.0**	**175.2**	47.4	**56.9**	46.2	**30.4**	637098	1020011	G57
93	**7.14**	**114.5**	**177.3**	**175.0**	**59.4**	**59.4**	**38.0**	**27.9**	650197	1024138	77
94	**8.14**	**123.1**	**179.8**	**177.3**	**59.4**	**59.4**	**27.9**	**28.5**	653075	903416	76
95	**8.46**	**127.4**	177.5	**175.3**	**51.2**	**55.0**	17.8	**41.8**	712969	767308	2
96	**7.23**	**108.6**	**174.9**	**171.6**	**62.0**	**55.6**	**44.3**	**31.7**	759883	1141307	G81
97	**8.41**	**125.9**	**176.9**	181.1	**52.5**	**63.8**	**19.0**	**32.3**	1246263	2151414	119
98	**7.75**	**130.2**	**176.4**	**182.6**	**54.4**	**52.5**	**20.3**	**19.7**	2090649	3027476	120

Results set for non-glycine/glycine pairs:

Resl	H#1	N#1	CO	CO#1	Cα#1	Cα	Cβ	Resp	Orig	Assign
0	**8.66**	**108.9**	**181.5**	**176.1**	**47.2**	**55.0**	**18.9**	26159	105340	51
1	**7.59**	**109.8**	**175.0**	**175.3**	**47.2**	**58.7**	**37.9**	30810	179360	78
2	**7.67**	**111.7**	**174.4**	**172.1**	**44.7**	**61.2**	**69.9**	31644	353981	117
3	**7.23**	**108.9**	**174.9**	**171.6**	**43.8**	**55.3**	**31.4**	42760	239490	81
4	**9.36**	**109.8**	**175.6**	**173.9**	**46.3**	**54.3**	**37.9**	52089	156349	91
5	**8.10**	**106.1**	**175.8**	**174.4**	**45.3**	**50.9**	**18.3**	133355	188283	102
6	**8.02**	**110.8**	**177.0**	**175.2**	**46.0**	**56.2**	**30.1**	199817	256557	57

Results set for glycine/non-glycine pairs:

Resl	H#1	N#1	CO	CO#1	Cα#1	Cα	Cβ#1	Resp	Orig	Assign
0	**8.23**	**126.8**	**176.1**	**179.1**	**59.6**	**47.2**	**32.0**	32508	180927	52
1	**8.45**	**118.5**	**177.8**	**173.6**	**54.3**	**44.1**	**41.0**	58575	153603	82
2	**7.74**	**120.6**	173.9	**177.3**	**54.3**	**46.3**	41.3	110568	162853	79
3	**7.93**	**121.2**	**175.0**	**176.1**	**64.0**	**47.2**	**30.7**	140608	254281	97
4	**7.86**	**113.9**	**175.2**	**176.6**	**58.7**	**46.0**	**64.3**	149052	236484	58