6 Appendix

6.1 Human VASP EVH1 domain

6.1.1 NH resonance assignment (kindly made available by L. J. Ball)

Res.Nr.	Res.	N-shift [ppm]	H_N-shift [ppm]
1	Met	122.19	8.55
2	Ser	117.17	8.22
3	Glu	119.80	8.00
4	Thr	117.07	8.92
5	Val	125.85	8.63
6	Ile	124.29	8.93
7	Cys	114.86	7.25
8	Ser	117.92	8.56
9	Ser	120.28	9.23
10	Arg	124.79	8.85
11	Ala	125.93	9.18
12	Thr	119.36	8.95
13	Val	128.22	8.28
14	Met	130.05	9.94
15	Leu	121.52	9.65
16	Tyr	125.39	8.13
17	Asp	128.67	8.11
18	Asp	124.12	8.33
19	Gly	106.96	8.34
20	Asn	116.04	7.30
20	Asn	116.98	8.33
20	Asn	116.98	6.84
21	Lys	118.58	7.67
22	Arg	114.12	6.98
23	Trp	121.88	8.71
23	Trp	130.04	10.10
24	Leu	123.51	9.12
26	Ala	126.24	8.41
27	Gly	110.90	8.92
28	Thr	111.83	8.69
29	Gly	109.58	8.52
31	Gln	122.59	8.48
31	Gln	111.40	7.44
31	Gln	111.40	6.65
32	Ala	127.28	8.86
33	Phe	118.43	8.57
34	Ser	115.32	8.83
35	Arg	122.60	8.58
36	Val	129.68	9.43
37	Gln	124.22	9.17
37	Gln	111.39	-
37	Gln	111.39	7.01
38	Ile	118.48	7.60
39	Tyr	127.02	9.49
40	His	121.78	9.54
41	Asn	126.04	8.51
41	Asn	112.67	7.72
41	Asn	112.67	6.94
43	Thr	114.19	7.73
44	Ala	121.98	6.96
45	Asn	117.08	7.89
45	Asn	110.23	7.64
45	Asn	110.23	6.62
46	Ser	109.47	7.55
47	Phe	120.13	9.39
48	Arg	119.10	8.91
49	Val	122.83	9.21
50	Val	125.24	8.88
51	Gly	116.08	9.05
52	Arg	123.65	8.13
53	Lys	125.43	9.18
54	Met	122.50	8.93
55	Gln	120.53	8.29
55	Gln	114.40	8.76
55	Gln	114.40	6.74
57	Asp	113.26	8.28
58	Gln	116.26	8.38
58	Gln	112.45	7.43
58	Gln	112.45	6.78
59	Gln	116.33	7.49
59	Gln	111.76	7.77
59	Gln	111.76	7.07
60	Val	127.32	8.79
61	Val	120.61	8.43
62	Ile	116.91	7.26
63	Asn	125.56	8.18
63	Asn	109.35	7.39
63	Asn	109.35	6.70
64	Cys	120.28	8.89
65	Ala	127.41	8.89
66	Ile	123.51	8.22
67	Val	118.41	6.84
68	Arg	120.02	8.49
69	Gly	113.90	9.05
70	Val	121.61	7.53
71	Lys	126.54	8.47
72	Tyr	128.24	8.76
73	Asn	127.06	9.14
73	Asn	110.80	7.25
73	Asn	110.80	6.79
74	Gln	125.74	8.78
74	Gln	111.80	7.35
74	Gln	111.80	6.80
75	Ala	129.83	7.75
76	Thr	109.94	8.79
78	Asn	109.74	7.85
78	Asn	111.11	7.28
78	Asn	111.11	6.70
79	Phe	123.29	7.91
80	His	126.28	8.09
81	Gln	115.62	8.82
81	Gln	109.00	-
81	Gln	109.00	6.57
82	Trp	119.78	9.10
82	Trp	128.20	9.97
83	Arg	120.05	8.47
84	Asp	126.62	8.94
85	Ala	121.39	8.52
86	Arg	117.00	8.64
87	Gln	119.85	8.62
87	Gln	113.03	7.49
87	Gln	113.03	6.70
88	Val	121.53	8.19
89	Trp	127.52	8.45
89	Trp	127.63	9.91
90	Gly	106.59	8.94
91	Leu	121.87	8.48
92	Asn	120.02	8.08
92	Asn	110.13	7.07
92	Asn	110.13	6.68
93	Phe	124.39	9.02
94	Gly	107.35	9.18
95	Ser	110.27	7.63
96	Lys	122.91	9.11
97	Glu	122.12	8.87
98	Asp	120.72	7.87
99	Ala	122.74	7.18
100	Ala	119.65	8.01
101	Gln	117.59	7.99
101	Gln	111.67	7.46
101	Gln	111.67	6.84
102	Phe	122.73	7.78
103	Ala	120.21	8.65
104	Ala	120.05	7.73
105	Gly	108.80	7.63
106	Met	121.96	8.12
107	Ala	120.10	7.95
108	Ser	114.17	7.62
109	Ala	126.23	7.58
110	Leu	115.44	8.02
111	Glu	118.79	7.88
112	Ala	122.31	7.52
113	Leu	117.49	7.79
114	Glu	118.59	7.62
115	Gly	113.44	7.60

6.2 Human VASP EVH2 domain

6.2.1 Resonance assignment

The assignments were deposited in the BioMagResBank under accession code 5955.

Residue	HN	Ha	Hβ	N	Cα	Cβ	Others
1Gly	8.16	4.02		108.71			
2Ser	8.11	4.78	3.94, 3.84	117.17	56.31	63.55	
3Pro	4.35		2.02		62.95	34.52	Hγ 1.85, Hδ 3.22
4Ser	8.77			117.80	58.67	63.96	
5Ser	8.51			117.89			
6Ser	8.42	4.52	3.90	117.80	58.73	63.87	
7Asp	8.37	4.63	2.69	122.46	54.67	41.24	
8Tyr	8.28	4.49	3.06	121.20	58.93	38.46	Hδ 7.09
9Ser	8.30	4.31	4.08, 3.95	116.76	59.78	62.32	
10Asp	8.48	4.54	2.79, 2.68	122.93	56.69	40.87	
11Leu	8.10	4.03	1.74, 1.56	120.46	58.02	41.72	Hδ 0.85
12Gln	8.02			117.34	58.60	27.87	
13Arg	7.93			120.21	59.48	29.48	
14Val	8.08	4.20	2.20	119.30	59.40	29.82	
15Lys	8.84	3.46	2.27	120.12	67.56	31.14	Hγ 1.00, Hδ 2.46, Hε4.03
16Gln	8.64	3.82	1.96	119.33	61.54	32.00	
17Glu	7.70	4.07	2.02	119.66	59.84	32.55	
18Leu	8.06	4.16	2.00	120.26	58.51	28.55	Hδ 0.87
19Leu	8.74	4.03	2.10, 1.47	119.78	57.75	41.72	Hδ 0.82
20Glu	7.93	3.91	2.24	118.12	58.68	27.68	
21Glu	7.53	4.14	2.06, 1.92	119.49	59.44	32.35	
22Val	8.11	3.81	2.20	118.46	66.36	31.57	Hγ 1.14
23Lys	8.34	3.74	2.26	121.02	60.36	31.28	
24Lys	7.95	3.95	2.28	116.59	59.61	29.19	Hδ 2.60
25Glu	8.22	4.08	2.27, 1.97	119.10	59.65	30.01	
26Leu	8.61	3.57	1.96	121.26	66.33	37.83	Hδ 0.85
27Gln	8.10	4.19	2.20, 1.90	118.77	61.83	32.71	
28Lys	7.82	4.36	1.98, 1.84	118.95	56.34	30.44	
29Val	7.64	4.19	1.94	119.20	57.56	37.17	Hγ1 1.67, Hγ2 1.49
30Lys	8.00	4.14	1.94	118.06	58.27	30.01	
31Glu	8.32	4.03	1.81, 1.50	119.27	60.41	31.39	
32Glu	7.92	4.01	2.24	117.41	58.81	28.20	Hγ 2.54
33Ile	8.40	4.07	2.00	119.60	59.32	30.01	Hδ10.86
34Ile	8.68	4.06	1.86	119.03	61.99	40.25	Hδ 10.88, Hγ1.66
35Glu	8.19	4.02	2.17, 2.01	118.11	59.31	29.30	Hγ 2.43
36Ala	7.86	4.24	1.68	120.32	55.10	18.59	
37Phe	8.30	4.20	3.03, 2.80	118.41	59.69	38.28	Hδ 6.44, Hε 6.85
38Val	8.58	3.37	2.15	121.11	67.34	34.87	Hγ 1.03
39Gln	8.32	4.00	2.17	117.26	58.89	28.13	Hγ 2.54
40Glu	7.98	4.13		118.76	58.75	29.14	
41Leu	8.32			119.12	57.55	41.58	
42Arg				118.04			
43Lys					57.88	32.82	
44Arg	7.86	4.39	2.01, 1.87	119.67	56.14	30.88	Hγ 1.77
45Gly	8.18	4.02		109.44			
46Ser	7.89	4.71	3.75	115.31			
47Pro							

6.2.2 Dihedral Angle restraints

These values are predictions from TALOS and based on chemical shifts.

Residue		ϕ	$\Delta\phi$	ψ	$\Delta\psi$
7	D	-85.0	15.0	138.0	21.0
8	Y	-82.0	20.0	132.0	18.0
9	S	-69.0	14.0	-28.0	20.0
10	D	-67.0	8.0	-35.0	10.0
11	L	-67.0	8.0	-39.0	10.0
12	Q	-65.0	5.0	-41.0	9.0
13	R	-62.69	6.16	-43.17	5.86
14	V	-69.15	4.19	-37.66	7.49
15	K	-62.76	5.65	-43.34	4.35
16	Q	-61.26	7.52	-41.26	9.33
17	E	-65.1	6.63	-41.56	8.39
18	L	-63.2	5.21	-4.89	5.84
19	L	-64.3	6.32	-43.79	6.75
20	E	-61.8	6.92	-37.87	7.86
21	E	-65.99	6.47	-42.4	3.15
22	V	-66.48	6.53	-38.74	6.92
23	K	-65.64	7.5	-37.55	11.44
24	K	-65.94	5.75	-37.37	5.38
25	E	-66.94	6.7	-41.38	7.43
26	L	-62.67	7.78	-41.53	7.67
27	Q	-63.35	6.99	-41.67	8.38
28	K	-61.72	5.37	-43.56	7.12
29	V	-76.22	16.92	-41.6	14.99
30	K	-69.0	2.0	-26.0	18.0
31	E	-67.69	1.54	-37.1	14.24
32	E	-72.26	9.15	-37.61	15.46
33	I	-64.21	5.64	-33.99	9.78
34	I	-67.81	6.95	-34.92	16.6
35	E	-66.5	8.47	-32.81	16.4
36	A	-63.77	7.21	-45.3	9.34
37	F	-65.97	4.15	-4.92	4.65
38	V	-68.44	7.99	-41.58	5.14
39	Q	-62.13	5.68	-36.67	1.6
40	E	-65.24	6.87	-44.33	9.5
41	L	-62.3	7.94	-43.35	9.88
42	R	-65.8	7.2	-4.9	8.68
43	K	-74.0	17.0	-24.0	14.0

6.2.3 H-Bond restraints

H-Bond restraints were introduced with an upper distance level of 2.2 Å, with an error of 1.5 Å, between the listed atoms.

15 O 19 HN
16 O 20 HN
17 O 21 HN
18 O 22 HN
19 O 23 HN
20 O 24 HN
21 O 25 HN
22 O 26 HN
23 O 27 HN
24 O 28 HN
25 O 29 HN
27 O 31 HN
28 O 32 HN
29 O 33 HN
30 O 34 HN
31 O 35 HN
32 O 36 HN
33 O 37 HN
34 O 38 HN
35 O 39 HN
36 O 40 HN
37 O 41 HN
38 O 42 HN

6.2.4 Residual Dipolar Couplings

All values are given in Hz, errors are given in brackets in the header of each table.

HN-N (0,3)	
1	-0.7
5	-4.7
6	-2.5
7	-5.4
8	5.8
9	4.3
10	9.5
13	20.3
14	-8.4
16	4.2
17	-4.4
18	-16.9
20	5.8
21	-0.6
22	2.2
24	2.0
25	6.9
26	3.7
27	-3.1
28	-1.0
29	-7.9
31	2.0
32	-0.5
33	1.8
34	1.9
35	-1.6
36	-2.4
37	10.0
38	-7.3
39	2.3
40	-1.7
41	2.7
42	7.4
46	-0.6

HN-Cα (1,8)	
5	-22.2
7	13.7
8	-34.2
9	9.9
10	-26.3
13	-55.5
14	86.8
16	25.0
17	42.0
18	3.4
20	29.3
21	-3.6
22	-92.8
23	-42.3
24	-27.8
25	-25.9
26	17.2
27	-6.1
28	-8.7
29	-14.4
31	-6.0
32	-2.8
33	25.4
34	-3.8
35	6.4
36	-11.2
37	-43.3
38	48.6
39	8.3
40	-17.2
41	16.2
42	21.9
43	22.4
45	-3.4
46	14.6

Hα-Cα (0,3)	
1	-6.4
5	-4.2
6	6.1
9	4.9
12	5.4
13	-14.7
15	-12.9
16	-3.9
18	5.9
19	14.7
20	5.3
21	9.0
23	3.9
25	-3.9
26	-5.6
27	4.8
28	2.5
32	3.9
35	-3.4
37	2.0
41	-3.1
42	6.2
43	-2.2
44	-2.5
46	-1.4

CO-Cα (2,5)	
1	-13.2
5	-8.8
6	-3.4
7	7.3
8	-2.8
9	3.3
10	33.2
13	-0.6
14	19.6
16	55.3
17	-32.2
18	0.9
20	23.9
21	21.2
22	-16.3
23	1.0
24	-17.1
25	3.8
26	-11.7
27	9.7
28	-7.6
29	5.7
31	-4.2
32	-1.3
33	4.9
34	17.4
35	13.2
36	1.0
37	5.3
38	-12.8
39	7.6
40	1.6
41	-10.3
42	1.1
43	6.6
45	9.6
46	7.8

N-CO (2,5)	
6	1.5
7	0.4
8	5.6
9	5.0
14	-10.2
16	-9.6
17	12.8
18	19.8
19	-11.3
20	-15.4
22	-8.5
23	-0.7
24	-16.0
25	8.2
26	2.4
27	11.7
28	-0.3
31	-3.0
32	-10.2
33	-3.9
34	5.1
35	7.5
37	20.0
38	-12.3
39	3.6
41	-1.9
42	17.6
43	-4.0
45	-17.4

6.3 Human Spred2 EVH1 domain

6.3.1 Resonance assignment

The assignments were deposited in the BioMagResBank under accession code 5939.
All values are given in ppm.

Residue	HN	Hα	Hβ	N	Cα	Cβ	CO	others
1 Gly					43.36			
2 Ser	8.71	4.72		115.91	58.32	63.90	170.31	
3 Met	8.63	4.51	2.10	122.33	55.79	32.64	174.67	HG1 2.64, HG2 2.52
4 Thr	8.16	4.72	4.26	114.94	61.92	69.49	176.48	CG2 21.74, HG2 1.18
5 Glu	8.35			123.22				
6 Glu	8.36	4.31	1.92	123.22	56.44	30.47	174.41	CG 36.25, HG 2.22
7 Thr	8.20	4.22	4.02	116.04	61.82	70.02	176.20	CG2 21.66, HG2 1.09
8 His	8.49	4.84	3.14 3.05	120.55	52.80	29.18	173.64	
9 Pro		4.22	2.11		63.17	32.29		CG 27.88, HD1 3.15 HD2 3.20, HG 1.53
10 Asp	8.67	4.55	2.70 2.62	122.60	54.10	41.21	176.71	
11 Asp	8.76	4.44	2.69	122.88	57.31	40.91	177.54	
12 Asp	8.48	4.56	2.70	117.84	55.28	40.35	177.79	
13 Ser	8.05	4.34	4.03 3.85	114.75	59.84	64.03	176.64	
14 Tyr	7.58	4.58	2.94 2.56	120.63	59.32	38.85	175.45	HD1 6.95, HE1 6.52, CD 120.40, HD 7.26 CE 117.34, HE 6.57
15 Ile	9.17	4.20	1.73	120.33	62.48	39.23	176.94	CG1 27.84, HG12 1.08, CG2 17.76 HG2 0.92, CD1 16.99, HD1 0.72
16 Val	7.42	4.44		116.50	60.46	33.14	176.15	HG1 0.88, HG2 0.87, CG 21.64
17 Arg	8.59	5.05	1.69 1.29	129.30	57.23	33.50	172.44	CG 27.45, HG1 1.25, HG2 0.93, CD 43.67 HD1 1.96, HD2 2.29
18 Val	9.25	4.89	2.43	118.39	58.85	36.73	174.45	CG1 21.74, HG1 1.03, CG2 18.61, HG2 0.95
19 Lys	8.69	5.26	1.71	121.22	55.39	33.12	174.40	CG 25.86, CD 29.36, HG 1.52
20 Ala	9.11	4.60	0.76	123.33	47.66	24.02	175.79	
21 Val	8.44	4.24	1.82	119.89	61.65	33.82	174.73	CG1 21.04, HG1 0.81, HG2 0.81, CG 21.24
22 Val	8.60	4.01	1.86	127.98	63.90	31.46	176.06	CG1 21.92, HG1 0.65, HG2 0.69, CG 22.26
23 Met	8.66	5.27	1.96 1.51	126.37	52.31	34.02	175.27	CG 32.30, HG1 2.16, HG2 2.59
24 Thr	9.44	4.67	3.73	117.20	60.11	70.98	175.09	CG2 20.41, HG2 0.89
25 Arg	7.91	3.80	-0.55 0.78	126.26	54.51	30.49	171.22	CG 26.65, HG1 0.44, HG2 -0.02, CD 42.52 HD1 1.93, HD2 2.03
26 Asp	8.67	4.60	2.50 2.77	126.60	52.59	41.91	175.32	
27 Asp	8.73	4.20	2.48	125.36	56.67	40.73	176.24	
28 Ser	8.36	4.25	3.88	114.79	60.58	62.92	177.47	
29 Ser	7.76	4.45	3.84	114.39	58.55	65.21	175.32	
30 Gly	8.21	3.46 4.03		112.08	45.70		175.87	
31 Gly	7.89	3.57 4.07		107.23	44.58		173.75	
32 Trp	8.08	4.97	2.52	119.69	55.94	31.22	171.49	NE1 129.38, HE1 9.84, CE3 122.22 HE3 7.06, CZ2 119.18, HZ2 5.61, CZ3 129. HZ3 6.23, CH2 132.40, HH2 7.05
33 Phe	9.21	4.98	2.77 3.02	120.52	55.79	40.57	175.91	HD1 6.57, HE1 6.88, CZ 124.46, HZ 6.62 CD 118.94, HD 6.45, CE 119.58, HE 6.91
34 Pro		4.90	1.80 1.69		63.00	31.82		CG 28.07, HG 2.08
35 Gln	8.56	4.17	1.80	125.57	49.74	29.97	176.89	CG 33.52, HG1 2.26, HG2 2.37, NE2 110.43 HE21 7.66, HE22 6.73
36 Glu	9.36	3.99	2.25 1.87	127.23	57.64	28.43	177.14	HG 2.28
37 Gly	8.35	3.69 4.21		108.72	45.57		176.51	
38 Gly	7.99	4.03 3.85		107.73	45.89		175.46	
39 Gly	8.16	4.22 3.79		108.76	44.10		174.13	
40 Ile	8.28	3.96	1.80	120.90	61.36	38.41	172.87	CG1 28.15, CG2 18.55, HG2 1.22, HD1 1.46 HG1 0.76
41 Ser	9.03	5.13	3.16 3.45	123.83	58.81	65.73	176.39	
42 Arg	8.75	4.92	1.58 1.77	121.14	55.75	31.21	172.67	CG 27.55, CD 43.78, HG 1.35, HD 3.02
43 Val	9.75	5.31	1.65	128.14	60.15	34.41	176.63	CG1 21.86, HG1 0.80, HG2 0.77, CG 22.12
44 Gly	8.82	5.03		111.35	46.68		173.92	

		4.65						
45 Val	7.70	5.04	1.61	118.97	60.53	33.33	170.63	CG1 21.36, HG1 0.24, CG2 21.36, HG2 0.26 CG 21.31
46 Cys	9.79	5.21	2.22 1.48	124.96	54.51	30.81	174.71	
47 Lys	8.14	4.25	1.47 1.59	123.33	56.00	33.77	172.68	CG 25.18, CD 29.33, CE 45.31, HG 1.04 HE 2.79
48 Val	8.03	4.18	1.83	122.47	60.47	34.36	175.67	CG1 20.11, HG1 0.68, CG2 20.09, HG2 0.68 CG 20.25 HG1 2.48, HG2 2.42
49 Met	8.47	4.42	1.83	123.91	54.95	32.29	175.01	
50 His	8.45	4.70	2.85 3.04	121.34	54.23	30.24	175.86	
51 Pro		4.28	2.09	64.19	31.90	50.75	27.32	HD1 3.47, HD2 3.24, HG 1.82
52 Glu	9.16	4.23	1.95	119.80	56.85	29.54	177.23	CG 36.47, HG 2.23
53 Gly	8.21	4.00 3.84		108.70	45.83		177.14	
54 Asn	8.39	4.54	2.76	118.58	53.50	38.38	174.48	ND2 112.34, HD21 7.50, HD22 6.77
55 Gly	8.39	3.95 3.73		107.73	45.49		175.60	
56 Arg	7.77	4.23	1.53 1.71	120.18	55.80	31.14	174.09	CG 27.21, CD 43.42, HD 3.05
57 Ser	8.24	4.69	3.73	117.27	57.92	65.04	175.82	
58 Gly	8.35	4.20 3.76		108.57	44.71		173.70	
59 Phe	8.97	5.49	2.61 2.44	117.72	56.96	44.00	172.07	HD1 6.89, HE1 7.13, CZ 129.75, HZ 7.33 CD 131.61, HD 6.88, CE 131.16, HE 7.15
60 Leu	9.18	4.65	1.10 1.52	124.10	53.28	47.11	173.36	CG 26.96, CD1 25.43, HD1 0.19, CD2 25.43 HD2 0.46
61 Ile	8.96	4.88	1.94	124.32	61.20	37.62	175.17	CG2 18.65, HG2 0.92
62 His	8.75	5.46	2.68 3.26	125.93	54.76	33.30	174.12	CD2 120.27, HD2 7.07, CE1 124.34 HE1 6.81
63 Gly	9.72	3.09 5.55		116.01	45.22		174.54	
64 Glu	8.53	5.13	1.78	122.70	53.39	33.75	170.82	HG 2.06
65 Arg	9.47	4.68	2.29 1.78	129.38	57.82	31.85	175.07	CG 27.38, CD 45.05, HD1 3.41, HD2 3.08
66 Gln	8.89	4.08	2.03	125.37	59.45	29.27	177.53	CG 34.70, NE2 111.22, HE21 7.36 HE22 6.94, HG 2.26
67 Lys	8.72	4.04	1.96 1.65	116.53	59.47	32.62	178.62	CG 24.46, CD 29.51, CE 45.48, HG 1.32 HE 2.92
68 Asp	7.54	4.66	2.45 2.96	113.52	52.29	41.24	176.99	
69 Lys	8.03	3.98	1.98	115.80	57.81	29.58	175.59	CG 24.40, CD 25.77, CE 42.08, HG 1.31 HD 1.59
70 Leu	7.21	4.14	1.55 1.45	120.01	55.86	43.25	174.84	CG 25.49, HG 1.35, CD1 26.92, HD1 0.79 CD2 26.78, HD2 0.88
71 Val	8.78	4.19	2.10	127.54	64.05	30.66	177.65	CG1 21.84, HG1 0.78, CG2 22.58, HG2 1.11
72 Val	7.70	4.38	2.29	120.82	60.55	33.05	176.35	CG1 22.13, HG1 0.83, CG2 18.51, HG2 0.65
73 Leu	7.31	4.51	1.24 1.62	122.86	55.47	46.41	174.51	CG 28.05, HG 0.72, HD2 0.81, CD 26.76
74 Glu	8.67	5.36	1.86 2.00	128.67	56.45	32.18	173.85	CG 37.32, HG1 2.17, HG2 2.08
75 Cys	8.75	4.92	2.57 2.71	122.10	55.86	30.08	174.37	
76 Tyr	9.04	4.65	2.81 3.02	126.13	60.14	38.34	172.85	HD1 7.15, HE1 6.69, CD 133.79, HD 7.26 CE 118.14, HE 6.72
77 Val	8.44	3.52	1.83	120.53	64.01	31.87	176.20	HG1 0.71, HG2 0.64, CG 22.56
78 Arg	6.23	4.81	2.15 1.67	121.15	53.09	35.22	174.43	CG 26.85, CD 43.25, HD1 3.37, HD2 3.24 HG 1.76
79 Lys	9.15	3.98	1.83	119.55	58.58	32.32	176.58	CG 25.21, CD 29.03, HG 1.51, HD 1.66
80 Asp	8.07	4.59	2.50 2.95	114.22	52.53	39.44	176.27	
81 Leu	7.14	4.52	1.79	122.03	57.50	43.52	175.56	CG 28.01, CD1 26.11, HD1 0.76, CD2 26.12 HD2 0.77, CD 26.06
82 Val	8.72	4.31	2.09	128.76	62.54	33.51	176.14	HG1 1.11, CG2 20.95, HG2 1.08, CG 21.07
83 Tyr	9.20	4.77	2.35 3.00	135.29	58.13	41.87	174.51	HD1 6.53, CD 132.59, HD 6.54, HE 7.30
84 Thr	9.44	4.15	2.44	127.24	62.26	69.94	174.62	CG2 21.39, HG2 0.77
85 Lys	8.62	4.09	1.07 1.63	127.50	54.79	29.41	172.25	CG 23.36
86 Ala	7.47	4.09	1.44	129.58	54.87	19.97	175.08	ND2 114.89, HD21 7.80, HD22 6.90
87 Asn	8.76	4.76	3.18	113.70	52.65	37.67	177.75	
88 Pro		4.47	2.48		65.97	32.82		CG 28.31, HG1 2.02 HG2 2.13
89 Thr	8.36	4.47	4.94	100.29	60.29	69.41	177.19	CG2 21.69, HG2 0.81
90 Phe	7.70	5.97	3.11 2.79	124.01	56.43	40.53	172.55	HD1 7.06, HE1 6.75, CZ 128.95, HZ 6.65 CD 114.93, HD 7.42, CE 120.99, HE 6.80
91 His	8.12	5.14	3.16 2.88	125.72	51.28	35.89	173.33	
92 His	8.48	4.97	2.84	116.09	54.16	34.06	172.32	
93 Trp	9.36	5.81	3.22 3.47	115.88	56.67	33.13	171.96	
94 Lys	8.69	5.79	1.83 1.75	121.06	54.50	36.45	174.31	CG 24.73, CD 29.89, HG 1.38
95 Val	9.17	4.60	1.31	124.36	61.16	34.24	175.76	CG1 22.62, CG2 19.90
96 Asp	9.55	4.31	3.08 2.84	129.31	56.21	40.12	173.43	
97 Asn	8.99	4.30	3.04 2.87	110.98	54.55	38.39		ND2 113.64 HD21 7.60, HD22 6.93

98 Arg	8.29	4.51	1.56 1.99	121.06	55.36	34.02	174.30	CG 27.38, CD 43.73, HD1 3.34, HD2 3.18 HG 1.80
99 Lys	7.86	5.25	1.47 1.69	119.15	55.14	35.08	173.98	CG 25.54, CD 29.60, HG 1.27, HD 1.51
100 Phe	8.22	4.83	0.68 2.21	119.72	56.20	44.07	175.15	HD1 7.07, HE1 7.35, CD 132.82, HD 6.97 CE 131.24, HE 7.37
101 Gly	7.76	4.33 2.91		104.40	45.05		173.22	
102 Leu	8.59	4.88	0.90 -0.15	119.43	53.50	46.95	170.77	CG 27.41, HG 0.64, HD1 0.07, HD2 0.07 CD 25.61, HD 0.06
103 Thr	8.53	5.25	3.88	115.54	61.05	69.48	174.63	CG2 22.08, HG2 1.85
104 Phe	9.12	4.52	3.48 2.30	126.19	57.59	41.97	175.23	HD1 6.63, HE1 7.19, HZ 7.46, HE 7.20
105 Gln	10.36 4.23	2.18		118.39	56.86	29.68	175.26	CG 34.64, HG1 2.37, HG2 2.32, NE2 111.70 HE21 7.34, HE22 6.84
106 Ser	7.40	5.03	3.87 4.20	109.12	54.98	65.06	176.02	
107 Pro		4.36	2.21 2.21		64.24	32.11		CG 27.78, HG1 2.22 HG2 1.87
108 Ala	8.03	3.98	1.40	120.99	55.03	18.05	179.00	
109 Asp	7.56	4.31	2.96 2.71	121.23	56.72	40.68	180.47	
110 Ala	6.81	1.71	0.74	122.21	53.82	20.40	176.96	
111 Arg	7.70	4.19	1.88 1.77	116.16	59.17	30.67	179.19	CG 27.90, CD 43.75, HD1 3.14, HD2 3.22 HG 1.54
112 Ala	7.77	3.96	1.45	121.82	54.84	17.62	179.20	
113 Phe	8.36	3.80	2.84 3.03	122.39	63.17	40.59	180.35	HD1 6.74, HE1 7.03, CZ 114.21, HZ 6.90 CD 123.10, HD 6.78, CE 119.30, HE 7.09
114 Asp	8.14	3.70	2.88	118.85	56.78	42.40	175.95	
115 Arg	7.90	3.61	1.72	116.13	59.54	29.83	177.25	CG 27.77, CD 43.31, HG 1.44, HD 3.05
116 Gly	7.80	3.11 3.59		108.06	46.69		178.94	
117 Val	7.94	2.86	1.50	122.73	67.16	30.42	173.98	CG1 21.81, HG1 0.27, CG2 23.95, HG2 -0.0
118 Arg	7.92	3.54	1.61	117.29	59.42	29.46	177.18	CG 27.59, CD 43.07, HG 1.40, HD 3.01
119 Lys	7.72	3.76	1.59 1.72	120.15	58.33	31.64	178.64	CG 24.42, HG1 1.16, HG2 1.23, CD 28.56 HD2 1.44, CE 45.46
120 Ala	7.31	2.54	0.65	120.51	54.32	18.57	176.96	
121 Ile	7.76	3.16	1.63	115.04	65.74	38.53	177.81	CG1 29.74, CG2 17.56, HG1 0.76
122 Glu	7.85	3.82	2.23 2.33	118.72	58.93	29.46	178.61	CG 36.42, HG 1.99
123 Asp	7.94	4.51	2.75 2.56	118.39	55.12	41.09	178.18	
124 Leu	7.50	4.32	1.89 1.58	122.27	55.84	42.94	177.36	CG 26.05, HG 1.04, HD1 0.94, HD2 0.91 CD 24.81
125 Ile	8.28	4.18	1.88	123.18	61.38	38.87	177.03	CG1 27.34, CG2 17.75, HG2 1.21, CD1 13.0 HD1 0.90, HG1 1.59
126 Glu	7.93	4.13	2.15 1.86	128.65	57.96	31.61	175.59	

6.3.2 Dihedral Angle Restraints

Values in degrees (°).

Residue			Bound		
			Upper	Lower	
4	THR	ϕ	-140	-100	**J**
6	GLU	ϕ	-114	-82	
6	GLU	ψ	123	155	
8	HIS	ϕ	-123	-57	
8	HIS	ψ	130	162	
11	ASP	ϕ	-71	-55	
11	ASP	ψ	-41	-25	
12	ASP	ϕ	-85	-63	
12	ASP	ψ	-44	-30	
13	SER	ϕ	-91	-57	
13	SER	ψ	-36	-10	
15	ILE	ϕ	-107	-71	
16	VAL	ψ	101	173	
17	ARG	ϕ	-139	-73	
17	ARG	ψ	97	167	
18	VAL	ϕ	-165	-81	
18	VAL	ψ	101	189	
19	LYS	ϕ	-140	-100	**J**
21	VAL	ψ	116	154	
22	VAL	ϕ	-96	-72	
22	VAL	ψ	118	140	
23	MET	ϕ	-122	-84	
23	MET	ψ	118	154	
24	THR	ϕ	-128	-86	
24	THR	ψ	126	146	
25	ARG	ϕ	-126	-64	
25	ARG	ψ	105	143	
26	ASP	ϕ	-117	-71	
26	ASP	ψ	103	139	
29	SER	ϕ	-140	-100	**J**
31	GLY	ϕ	-116	-62	
31	GLY	ψ	101	165	
32	TRP	ϕ	-140	-100	**J**
33	PHE	ϕ	-140	-100	**J**
36	GLU	ϕ	-124	-52	
36	GLU	ψ	117	169	
40	ILE	ϕ	-105	-71	
40	ILE	ψ	94	158	
41	SER	ϕ	-109	-71	
41	SER	ψ	119	137	
42	ARG	ψ	120	150	
43	VAL	ϕ	-129	-81	
43	VAL	ψ	119	173	
45	VAL	ϕ	-130	-68	
45	VAL	ψ	129	191	
46	CYSS	ϕ	-140	-100	**J**
48	VAL	ϕ	-132	-64	
48	VAL	ψ	103	167	
49	MET	ϕ	-117	-65	
49	MET	ψ	105	147	
50	HIS	ϕ	-101	-75	
50	HIS	ψ	121	165	
54	ASN	ϕ	-140	-100	**J**
54	ASN	ψ	-41	9	
57	SER	ϕ	-138	-114	
57	SER	ψ	151	187	
59	PHE	ϕ	-151	-117	
59	PHE	ψ	139	165	
60	LEU	ϕ	-141	-121	
60	LEU	ψ	108	148	
61	ILE	ϕ	-140	-100	**J**
63	GLY	ϕ	-140	-100	**J**
64	GLU	ψ	128	152	
65	ARG	ψ	120	144	
66	GLN	ϕ	-81	-53	
66	GLN	ψ	-54	-16	
67	LYS	ϕ	-92	-62	
67	LYS	ψ	-46	-12	
68	ASP	ϕ	-116	-70	
68	ASP	ψ	-21	11	
70	LEU	ϕ	-104	-64	
70	LEU	ψ	119	149	
72	VAL	ϕ	-140	-100	**J**
73	LEU	ϕ	-165	-115	
73	LEU	ψ	114	148	
74	GLU	ϕ	-149	-111	
74	GLU	ψ	114	138	
75	CYSS	ϕ	-134	-94	
76	TYR	ϕ	-117	-55	
76	TYR	ψ	120	148	
78	ARG	ϕ	-159	-113	
78	ARG	ψ	140	174	
79	LYS	ϕ	-86	-70	
80	ASP	ϕ	-140	-100	**J**
80	ASP	ψ	-4	20	
81	LEU	ϕ	-100	-68	
81	LEU	ψ	101	149	
82	VAL	ϕ	-140	-100	**J**
82	VAL	ψ	113	141	
83	TYR	ϕ	-138	-80	
83	TYR	ψ	117	139	
84	THR	ϕ	-114	-72	
84	THR	ψ	113	139	
85	LYS	ϕ	-118	-52	
85	LYS	ψ	94	158	
89	THR	ϕ	-140	-100	**J**
89	THR	ψ	-57	-13	
91	HIS	ϕ	-140	-100	**J**
92	HIS	ϕ	-152	-102	
93	TRP	ϕ	-157	-101	
93	TRP	ψ	129	177	
94	LYS	ϕ	-113	-71	
94	LYS	ψ	104	136	
98	ARG	ϕ	-140	-72	
98	ARG	ψ	131	167	
99	LYS	ϕ	-142	-96	
99	LYS	ψ	114	154	
100	PHE	ϕ	-150	-118	
100	PHE	ψ	119	179	
102	LEU	ϕ	-152	-88	
102	LEU	ψ	129	157	
103	THR	ϕ	-127	-87	
103	THR	ψ	110	136	
104	PHE	ϕ	-125	-81	
104	PHE	ψ	120	154	
105	GLN	ϕ	-112	-80	
105	GLN	ψ	-32	8	
106	SER	ϕ	-132	-100	
106	SER	ψ	131	171	
108	ALA	ϕ	-70	-58	
108	ALA	ψ	-47	-31	
109	ASP	ϕ	-73	-57	
109	ASP	ψ	-55	-21	
110	ALA	ϕ	-73	-51	
110	ALA	ψ	-41	-29	
111	ARG	ϕ	-78	-66	
111	ARG	ψ	-45	-27	
112	ALA	ϕ	-71	-61	
112	ALA	ψ	-45	-39	
113	PHE	ϕ	-68	-58	
113	PHE	ψ	-49	-37	
114	ASP	ϕ	-69	-57	
114	ASP	ψ	-51	-29	
115	ARG	ϕ	-74	-58	
115	ARG	ψ	-46	-34	
116	GLY	ϕ	-69	-59	
116	GLY	ψ	-43	-35	
117	VAL	ϕ	-71	-59	
117	VAL	ψ	-48	-24	
118	ARG	ϕ	-71	-57	
118	ARG	ψ	-47	-23	
119	LYS	ϕ	-82	-62	
119	LYS	ψ	-53	-19	
120	ALA	ϕ	-77	-53	
120	ALA	ψ	-40	-26	
121	ILE	ϕ	-84	-64	
121	ILE	ψ	-48	-28	

J: value from J coupling measurement, used if TALOS was different or bad prediction

6.3.3 H-Bond restraints

Hydrogen-bonds for α-helix, res. 108-126

HN 110 O 106
HN 111 O 107
HN 112 O 108
HN 113 O 109
HN 114 O 110
HN 115 O 111
HN 116 O 112
HN 117 O 113
HN 118 O 114
HN 119 O 115
HN 120 O 116
HN 121 O 117
HN 122 O 118
HN 123 O 119
HN 124 O 120
HN 125 O 121

Hydrogen-bonds for β-sheets

HN 18 O 43
HN 43 O 18
HN 20 O 41
HN 41 O 20
HN 92 O 84
HN 84 O 92
HN 93 O 100
HN 100 O 93
HN 94 O 82
HN 82 O 94