Table I. Free energies in Kcal/mol for the intrinsic tendencies of the different amino acids to be at different positions of an a-helix.

	Nc-1	Nc-2	Nc-3	Nc-4	Cc-1	Cc-2	N1	N2	N3	N4	Ncen	Neutral
P	0.50	0.50	0.50	0.50	0.82	0.82	0.88	2.48	3.13	3.13	3.13	
G	-0.30	-0.30	-0.30	-0.30	0.00	0.00	1.51	1.28	1.51	1.81	1.81	
A	0.40	0.30	0.40	0.30	0.40	0.40	0.68	0.68	0.68	0.68	0.68	
C	-0.20	-0.30	-0.50	-0.50	0.20	-0.40	1.18	1.18	1.28	1.28	1.28	1.28
S	-0.70	-0.85	-0.65	-0.90	0.40	0.40	1.10	1.23	1.38	1.23	1.20	
T	-0.50	-0.70	-0.60	-0.90	0.75	0.95	1.18	1.18	1.33	1.41	1.51	
N	-0.65	-0.70	-0.65	-0.90	-0.00	-0.35	1.28	1.38	1.38	1.48	1.28	
D	-0.40	-0.50	-0.70	-0.90	0.40	0.40	1.18	1.28	1.40	1.40	1.40	1.40
Q	0.70	0.60	0.70	0.60	0.00	0.00	0.93	0.93	0.88	0.96	1.03	
E	0.20	0.10	0.20	0.10	0.40	0.40	0.83	0.83	0.98	1.08	1.08	0.87
K	0.40	0.30	0.40	0.30	0.00	0.00	0.83	0.83	0.83	0.83	0.83	0.72
R	0.40	0.40	0.40	0.30	0.00	0.00	0.74	0.74	0.74	0.74	0.74	0.62
H	-0.00	-0.00	-0.00	-0.00	0.40	0.00	1.48	1.48	1.48	1.48	1.48	1.33
L	0.40	0.30	0.40	0.30	0.40	0.40	0.83	1.08	0.98	0.83	0.83	
I	0.40	0.30	0.40	0.30	0.75	0.75	0.96	1.08	1.08	0.91	1.08	
V	0.40	0.30	0.40	0.30	0.50	0.50	1.03	1.13	1.18	1.18	1.30	
M	0.40	0.30	0.40	0.30	0.40	0.40	0.84	1.04	1.14	0.94	0.94	
F	0.40	0.30	0.40	0.30	0.00	-0.30	1.13	1.13	1.23	1.23	1.23	
Y	0.20	0.20	0.40	0.30	0.00	-0.30	1.13	1.13	1.23	1.23	1.23	1.23
W	0.00	-0.10	0.40	0.30	0.40	0.00	1.13	1.13	1.23	1.23	1.23	
Ac	-0.70	-0.70	-0.70	-0.70								
Am					-0.10	-0.10						

The first column corresponds to the 20 amino acids in one lettter. The N-terminus blocking acetyl or succynil groups are indicated by Ac and the C-terminus blocking amide group by Am.

Nc-1 Normal N-cap values.

Nc-2 N-cap values when there is a Pro at position N1.

Nc-3 N-cap values when there is a Glu, Asp or Gln at position N3.

Nc-4 N-cap values when there is a Pro at position N1 and Glu, Asp or Gln at position N3.

Cc-1	Normal C-cap values.
Cc-2	C-cap values when there is a Pro residue at position C'.
N1	Intrinsic helical propensities at position N1.
N2	Intrinsic helical propensities at position N2.
N3	Intrinsic helical propensities at position N3.
N4	Intrinsic helical propensities at position N4.
Ncen	Intrinsic helical propensities between N4 and C-cap.
	For charged residues these could change depending of the degree of ionisation.
Neutral	Intrinsic helical propensities at positions higher than N4.

Table II. Energy contributions in Kcal/mol * 100, of the interactions between different amino acids at positions N' (rows) and N4 (columns) in a hydrophobic staple motif.

N' \ N4	P	G	A	C	S	T	N	D	Q	E	K	R	H	L	I	V	M	F	Y	W
P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	0	0	0	0	0	0	0	0	0	-30	-10	-10	-30	0	0	0
C	0	0	0	0	0	0	0	0	0	0	0	0	0	-30	-10	-10	-30	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
T	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D	0	0	0	0	0	0	0	0	0	0	-30	-30	-30	0	0	0	0	0	0	0
Q	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
E	0	0	0	0	0	0	0	0	0	0	-30	-30	-30	0	0	0	0	0	0	0
K	0	0	0	0	0	0	0	-30	0	-30	0	0	0	-30	-30	-30	-30	-30	-10	-20
R	0	0	0	0	0	0	0	-30	0	-30	0	0	0	-30	-30	-30	-30	-30	-10	-20
H	0	0	0	0	0	0	0	-30	0	-30	0	0	0	0	0	0	0	0	0	0
L	0	0	-65	-60	0	0	0	0	0	0	-60	-60	0	-90	-30	-40	-60	-40	-40	-40
I	0	0	-35	-30	0	0	0	0	0	0	-30	-30	0	-75	-90	-70	-40	-40	-40	-40
V	0	0	-30	-25	0	0	0	0	0	0	-30	-30	0	-60	-70	-40	-40	-20	-20	-20
M	0	0	-65	-60	0	0	0	0	0	0	-30	-30	0	-90	-30	-40	-60	-40	-40	-40
F	0	0	-30	-25	0	0	0	0	0	0	-30	-30	0	-70	-70	-70	-70	-40	-40	-40
Y	0	0	-20	-15	0	0	0	0	0	0	-30	-30	0	-40	-70	-70	-70	-40	-40	-40
W	0	0	-20	-15	0	0	0	0	0	0	-30	-30	0	-40	-70	-70	-70	-40	-40	-40

The hydrophobic staple motif is only considered whenever the N-cap residue is Asn, Asp, Ser, Pro or Thr. The above values are multiplied by 1 in the following cases: *i)* whenever the N-cap residue is Asn, Asp, Ser, or Thr and the N3 residue is Glu, Asp or Gln. *ii)* whenever the N-cap residue is Asp or Asn and the N3 residue is Ser or Thr. In all other cases they are multiplied by 0.5.

Table III. Energy contributions in cal/mol Kcal/mol * 100 of the interactions between the different amino acids at positions C3 (rows) and C' (columns), in the Schellman motif.

	P	G	A	C	S	T	N	D	E	Q	K	R	H	L	I	V	M	F	Y	W
P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-30	-10	-10	-10	0	0
C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
T	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D	0	0	0	0	0	0	0	0	20	20	0	-20	-20	0	0	0	0	0	0	0
Q	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
E	0	0	0	0	0	0	0	0	20	20	0	-20	-20	0	0	0	0	0	0	0
K	0	0	0	0	0	0	0	0	-20	-20	0	0	0	0	-30	-10	-10	-10	0	0
R	0	0	0	0	0	0	0	0	-20	-20	0	0	0	0	0	0	0	0	0	0
H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
L	0	0	0	-10	0	0	0	0	0	0	0	0	0	-10	-10	-15	-10	-10	-20	-10
I	0	0	0	-10	0	0	0	0	0	0	0	0	0	0	-25	-10	-10	-10	-10	-10
V	0	0	0	-10	0	0	0	0	0	0	0	0	0	0	-10	-10	-10	-10	-10	-10
M	0	0	0	-10	0	0	0	0	0	0	0	0	0	0	-30	-10	-10	-10	-10	-10
F	0	0	-30	0	0	0	0	0	0	0	-30	0	0	0	-15	-10	-10	-10	0	0
Y	0	0	0	0	0	0	0	0	0	0	-30	0	0	0	-10	-10	-10	-10	0	0
W	0	0	0	0	0	0	0	0	0	0	-30	0	0	0	-10	-10	-10	-10	0	0

The Schellman motif is only considered whenever Gly is the C-cap residue.

Table IV. Energy contributions in cal/mol Kcal/mol * 100 of the non-charged side chain-side chain interactions between the different amino acids at positions i,i+3 (first row) and i,i+4 (second row).

	P	G	A	C	S	T	N	D	Q	E	K	R	H	L	I	V	M	Y	F	W
P	0	0	0	0	0	0	0	0	0	0	0	0	0	-20	-20	-20	-20	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0	-20	-20	-20	-20	-20	-20	-20
G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	10	10	0	10	10	10	10	15	15	15
A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	20	20	20	20	0	0	-20	-20	-40	20	20	20	20	-60	-60	-60
S	0	0	0	0	0	0	0	0	0	0	10	10	0	0	0	0	0	-0	-0	-0
	0	0	0	0	20	10	20	20	0	0	10	10	0	0	0	0	0	15	15	15
T	0	0	0	0	0	0	0	0	10	10	20	20	0	0	-20	0	0	0	0	0
	0	0	0	0	10	0	10	10	0	0	0	0	0	-20	-10	-10	-20	15	15	15
N	0	0	0	0	0	0	0	0	20	20	0	0	0	0	0	0	0	0	-20	0
	0	0	0	20	20	10	20	20	0	0	10	10	0	0	0	0	0	-20	-20	-20
D	0	0	0	0	0	20	0	0	0	-0	-5	-30	-0	0	0	0	0	15	15	15
	0	0	0	0	20	10	20	20	-15	-15	-15	-30	-8	0	0	0	0	0	0	0
Q	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-0	0	-0
	0	0	0	0	0	-20	-60	-40	-15	-20	0	0	-5	-15	-15	-15	-15	-20	-20	-20
E	0	0	0	0	0	0	0	0	0	0	-15	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	-30	-30	0	-40	-20	-45	-0	-15	-15	-15	-15	20	20	20
K	0	0	0	0	0	0	0	5	0	-15	15	15	0	-10	0	0	0	-0	0	0
	0	0	0	0	0	0	0	-40	0	-10	10	10	20	-15	-15	-15	-15	-20	-20	-20
R	0	0	0	0	0	0	0	20	-15	-35	0	0	0	-10	0	0	0	-0	0	0
	0	0	0	0	0	0	0	-20	0	-40	0	0	0	-15	-15	-15	-10	-20	-20	-20
H	0	0	0	0	0	0	0	0	0	0	0	20	0	-00	-00	-00	-00	-0	-0	-0
	0	0	0	0	0	0	0	-30	-0	0	20	20	40	-0	-00	-00	-00	-30	-30	-30
L	0	0	0	0	20	0	15	15	0	0	0	0	0	-35	-43	-30	-30	-20	-20	-20
	0	0	0	0	20	20	20	20	0	15	0	0	0	-50	-57	-50	-30	-30	-30	-30
I	0	0	0	0	0	0	20	30	0	15	0	0	0	-26	-30	-20	-30	-30	-30	-30
	0	0	0	0	30	20	30	30	0	0	0	0	80	-40	-30	-30	-30	40	40	40
V	0	0	0	0	0	0	20	30	0	15	0	0	0	-20	-30	-20	-30	-10	-30	-30
	0	0	0	-30	20	20	30	30	0	0	0	0	80	-44	-30	-30	-30	40	40	40
M	0	0	0	0	0	0	0	0	0	0	0	0	0	-30	-10	-10	-20	-30	-30	-30
	0	0	0	0	20	20	20	20	0	15	0	0	0	-40	-30	-30	-40	-40	-40	-40
F	0	0	0	0	0	0	0	0	0	0	-0	-0	-25	0	-30	-20	-30	-45	-45	45
	0	0	0	-80	10	-30	-50	30	-30	0	-20	-20	-40	-40	-60	-30	-70	-80	-80	-80
Y	0	0	0	0	0	0	0	0	0	0	0	0	-25	0	-30	-20	-30	-45	-45	45
	0	0	0	-80	10	-30	-50	30	-50	0	-20	-20	-60	-40	-40	-30	-60	-80	-80	-80

W	0	0	0	0	0	0	0	0	0	0	-0	0	-25	0	-30	-30	-30	-45	-45	45
	0	0	0	-80	10	-30	-50	30	-30	0	-20	-20	-40	-30	-30	-30	-60	-80	-80	-80

The interaction free energies correspond to those between non-charged residues, or in the case of two residues that can be charged to those cases in which at least one of the two is non-charged (the interaction is scaled according to the population of charged and neutral forms of the participating amino acids).

Table V. Side chain interactions involving at least one charged side chain that are pH dependent but not affected by ionic strength.

Position i	Position i+4	Kcal/mol
Phe,Tyr,Trp	His^+	-0.4[a]
Gln	Asp^-	-0.5[b]
Glu^-	Asn	-0.5[c]
Gln	Glu^-	-0.1[c]

This interaction energy is to be added to that shown in Table IV when one of the residues in the pair becomes charged. [a]These numbers have been obtained after fitting AGADIR1s-2 to the reference poly-alanine based peptides from Armstrong *et al*, (1993b). This value is appropriate when His is at position C1 or C-cap, otherwise it should be divided by three (see Results section). [b]These numbers have been obtained after fitting AGADIR1s-2 to the reference poly-alanine based peptides from Huyghues-Despointes *et; al* (1995). [c]This work based on the analysis of our peptide database.

Table VI. Average distance between charged groups (Å).

Pos	i+1	i+2	i+3	i+4	i+5	i+6	i+7	i+8	i+9	i+10	i+11	i+12
Helix												
DD	5.5	7.3	5.5	6.5	9.8	11.2	10.7	13.0	14.8	15.7	16.0	19.0
DE	5.8	8.6	6.4	7.0	10.5	11.9	10.7	14.6	14.8	15.9	16.1	19.0
DK	7.3	10.5	6.2	7.0	11.4	11.8	10.4	15.0	17.1	17.4	17.6	20.0
DR	7.2	11.7	5.8	5.4	11.9	11.7	10.8	15.0	15.1	16.2	18.6	22.6
ED	7.2	11.8	7.3	7.2	11.8	12.1	12.0	14.8	16.1	16.2	22.5	22.5
EE	7.3	10.6	7.6	7.8	12.1	12.1	11.2	12.8	17.4	17.2	20.3	20.0
EK	9.5	12.1	6.5	5.9	15.0	13.7	13.3	13.8	18.4	17.5	18.0	20.9
ER	9.6	11.6	6.5	4.9	15.5	14.3	13.3	14.4	19.4	14.8	16.6	19.6
KD	8.0	12.5	7.5	7.0	12.0	13.0	13.8	15.0	18.0	15.8	18.2	20.0
KE	7.4	11.1	7.2	5.9	12.0	13.4	12.2	17.0	17.0	17.0	17.7	17.6
KK	10.0	12.6	8.8	8.2	12.0	14.3	11.4	16.0	18.0	16.9	18.2	21.4
KR	10.0	12.7	7.0	8.5	13.3	13.6	13.2	16.8	17.3	18.0	15.8	21.0
RD	7.4	11.0	7.5	5.4	13.3	13.6	11.9	17.8	17.7	18.0	18.0	21.0
RE	8.5	12.6	7.8	4.9	13.7	14.6	11.8	16.4	17.1	19.4	19.5	20.9
RK	9.7	13.2	8.6	8.0	14.7	15.0	13.8	16.4	20.6	18.3	19.7	22.0
RR	10.0	13.2	8.6	8.0	14.7	15.3	12.2	13.3	21.3	18.9	16.8	19.5
DH	8.2	10.5	8.5	8.3	10.4	13.0	10.8	12.8	17.4	17.2	20.3	20.0
EH	10.0	11.0	7.5	8.7	12.3	15.2	11.5	14.3	17.4	17.2	20.3	20.0
KH	10.0	10.9	8.0	7.8	13.2	13.9	12.7	15.2	17.4	17.2	20.3	20.0
RH	9.3	12.7	8.9	9.3	13.7	15.4	11.1	16.1	17.4	17.2	20.3	20.0
HD	7.0	8.8	5.5	5.5	10.4	11.1	10.4	11.9	17.4	17.2	20.3	20.0
HE	6.5	9.4	6.6	6.5	10.9	12.5	10.9	13.1	17.4	17.2	20.3	20.0
HK	9.6	11.3	7.0	6.9	12.5	13.5	8.7	13.5	17.4	17.2	20.3	20.0
HR	10.3	12.0	7.4	8.0	14.5	15.0	9.9	10.1	17.4	17.2	20.3	20.0
HelixRest	10.6	9.6	7.2	7.2	14.7	14.3	9.1	12.7	19.0	17.8	20.3	23.0
Ncap	7.7	7.0	5.9	11.2	11.2	14.5	15.4	15.9	18.0	20.0	20.7	23.0
N′	10.7	10.8	12.3	5.7	7.1	13.0	12.1	9.6	12.4	16.4	14.1	13.5
Ccap	10.7	9.6	9.0	9.0	15.1	13.6	12.5	16.6	19.2	17.3	18.5	22.8
C′	10.7	9.6	15.4	13.6	18.2	21.0	20.0	20.2	24.5	25.4	24.7	27.1

C'G-cap	10.7	6.8	13.0	12.1	4.75	9.51	14.8	11.8	8.43	15.2	17.5	14.2
N-cap f	9.3	9.2	7.5	5.4	12.0	11.1	10.5	14.2	16.1	15.3	16.9	18.0
N' f	10.7	9.6	12.4	5.1	11.2	15.4	12.2	11.3	17.1	18.5	15.2	18.4
C-cap f	8.03	9.6	9.46	7.36	12.7	14.7	12.8	14.4	18.3	18.7	18.2	21.0
C' f	10.7	9.6	12.0	9.10	7.40	12.5	14.3	10.2	11.9	17.3	17.0	14.9
R.Coil												
DD	6.0	7.0	8.1	10.4	12.3	14.1	15.5	16.5	18.7	19.5	20.5	21.7
DE	6.8	8.0	8.5	9.9	12.3	13.6	15.5	16.5	18.7	19.5	20.5	21.7
DK	8.6	11.0	9.0	10.6	12.8	13.8	15.8	17.5	18.6	19.6	20.5	21.7
DR	8.4	8.2	9.0	9.6	13.0	13.6	15.8	16.8	18.6	19.6	20.5	21.7
ED	8.0	10.5	10.3	12.1	15.0	15.2	15.8	17.3	19.7	19.7	20.5	22.0
EE	7.9	9.4	10.1	10.8	15.0	15.9	16.4	17.9	19.6	19.7	20.5	20.8
EK	7.8	10.5	10.0	11.4	14.0	16.0	17.0	17.4	18.6	19.6	20.5	21.7
ER	10.8	10.2	9.5	10.7	14.0	15.6	16.6	16.7	20.0	20.8	21.5	21.7
KD	8.3	11.0	10.7	11.5	16.2	15.8	17.0	19.3	21.0	19.8	21.5	23.6
KE	9.1	10.4	11.8	11.0	16.2	16.6	17.4	18.7	19.3	20.9	21.5	23.0
KK	11.6	12.6	13.1	15.0	16.0	16.8	17.4	18.3	20.6	21.4	22.5	23.7
KR	11.3	12.7	13.2	15.0	15.6	17.6	17.4	18.0	19.3	22.5	22.5	23.5
RD	9.5	10.3	7.9	12.7	14.5	15.7	17.4	18.3	21.1	20.3	21.5	22.2
RE	9.3	10.4	11.4	11.0	14.3	15.3	17.4	17.8	19.2	20.6	21.5	21.9
RK	11.3	14.0	13.6	15.0	14.8	18.0	18.5	18.9	20.0	22.3	22.5	22.5
RR	12.0	12.0	13.0	15.0	16.7	17.0	18.0	18.1	20.3	21.5	22.0	22.3
DH	7.2	7.9	9.0	9.9	11.9	13.7	14.5	17.6	19.2	20.6	21.5	21.9
EH	8.2	8.8	11.3	10.6	11.6	15.3	17.6	17.4	19.2	20.6	21.5	21.9
KH	9.1	10.4	11.8	12.9	13.9	16.8	16.9	18.0	19.2	20.6	21.5	21.9
RH	8.6	10.2	11.6	12.1	12.1	16.1	19.2	18.2	19.2	20.6	21.5	21.9
HD	7.0	8.2	9.6	10.5	13.0	14.4	16.5	17.5	19.2	20.6	21.5	21.9
HE	6.9	8.3	9.6	11.2	13.3	14.8	15.4	17.9	19.2	20.6	21.5	21.9
HK	11.8	11.5	11.2	12.3	14.6	15.0	16.2	20.4	19.2	20.6	21.5	21.9
HR	9.4	10.5	10.7	10.7	12.9	16.5	15.4	18.2	19.2	20.6	21.5	21.9
RcoilRest	10.7	9.6	13.2	13.2	19.6	19.9	25.4	26.5	31.5	33.1	37.7	39.0

The distances shown in this table have been obtained from the analysis of the protein database, or from a modeled helix, as indicated in Methods and represent average values. In the different columns we show the distance between residues at position i and i+x. The amino acid pairs are shown in one-letter code. The

nomenclature for the helix position of the charged residues (columns N-cap etc...) is that of Richardson & Richardson (1988).

Helix	Distance between i i+x pairs of charged residues located inside an a-helix (excluding caps).
Helixrest	The same but for all possible charged pairs not included before.
Ncap	Distance between the N-cap residue (i) and a helical residue located at position i+x.
N'	Distance between the residue at position N' (i) and a helical residue located at position i+x.
Ccap	Distance between the C-cap residue (i) and a helical residue located at position i-x.
C'	Distance between residue C' (i) when residue C' is not a Gly and a helical residue located at position i-x.
C'gcap	Distance between residue C' (i) when residue C' is a Gly and a helical residue located at position i-x. The presence of a Gly allows dihedral angles forbidden, or not favourable, for other residues and therefore affects to the distance between a charged group at position C' and the helix charged residues.
N-cap f	Distance between the free N-terminal group when this group is located at the N-cap position and a helical residue at position i+x.
N' f	Distance between the free N-terminal group, when this group is located at position N', and a helical residue at position i+x.
C-cap f	Distance between the free C-terminal group, when this group is located at the C-cap position, and a helical residue at position i-x.
C' f	Distance between the free C-terminal group, when this group is located at position C', and a helical residue at position i-x.
Rcoil	Distance between i, i+x pairs of charged residues in the whole protein database.
RcoilRest	Average distance between i, i+x pairs of charged residues in the reference state not included in Rcoil.

Table VII. Distances (Å) between charged amino acids and the half charge from the helix macrodipole.

Res	N-cap	N1	N2	N3	N4	N5	N6	N7	N8	N9	N10	N11	N12	N13
Glu	7.0	6.1	7.5	7.7	7.9	9.8	10.6	11.1	12.4	13.8	14.5	16.0	17.5	20.0
Asp	5.0	6.0	6.0	6.0	8.9	10.0	10.5	11.0	11.5	12.9	14.5	16.0	17.5	20.0
Lys	9.5	9.7	9.7	7.7	9.7	10.1	11.4	12.6	13.9	14.5	15.5	16.0	17.5	20.0
Arg	9.5	9.7	9.7	7.7	9.7	10.1	11.4	12.6	13.9	14.5	15.5	16.0	17.5	20.0
His	4.0	6.1	8.0	8.7	9.0	9.8	10.6	11.1	12.4	13.8	14.5	16.0	17.5	20.0
Cys	5.0	6.0	6.0	5.0	8.9	10.0	10.5	11.0	11.5	12.9	14.5	16.0	17.5	20.0
Tyr	7.0	6.1	7.5	7.7	7.9	9.8	10.6	11.1	12.4	13.8	14.5	16.0	17.5	20.0
Res	C-cap	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13
Glu	9.8	9.4	9.4	9.4	9.1	10.1	11.4	12.6	13.9	14.4	15.5	16.0	17.5	20.0
Asp	8.0	8.0	9.4	9.4	9.1	10.1	11.4	12.6	13.9	14.5	15.5	16.0	17.5	20.0
Lys	6.3	7.3	7.5	7.7	8.4	11.4	12.9	12.8	14.0	14.9	16.7	17.9	19.3	20.0
Arg	6.3	7.3	7.5	7.7	8.4	11.4	12.9	12.8	14.0	14.9	16.7	17.9	19.3	20.8
His	4.5	4.5	8.0	8.7	10.5	11.4	12.9	12.8	14.0	14.9	16.7	17.9	19.3	20.8
Cys	7.0	7.0	7.2	7.5	9.1	10.1	11.4	12.6	14.0	14.5	15.5	16.0	17.5	20.0
Tyr	9.8	9.4	9.4	9.4	9.1	10.1	11.4	12.6	13.9	14.5	15.5	16.0	17.5	20.0

The distances in Å shown in this table have been obtained from the analysis of the protein database as indicated in Methods. The nomenclature for the helix position of the charged residues (columns N-cap etc...) is that of Richardson & Richardson (1988).