Supplementary data for the article:

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Supporting Information

C–H/O interactions of aromatic CH donors within proteins: a crystallographic study

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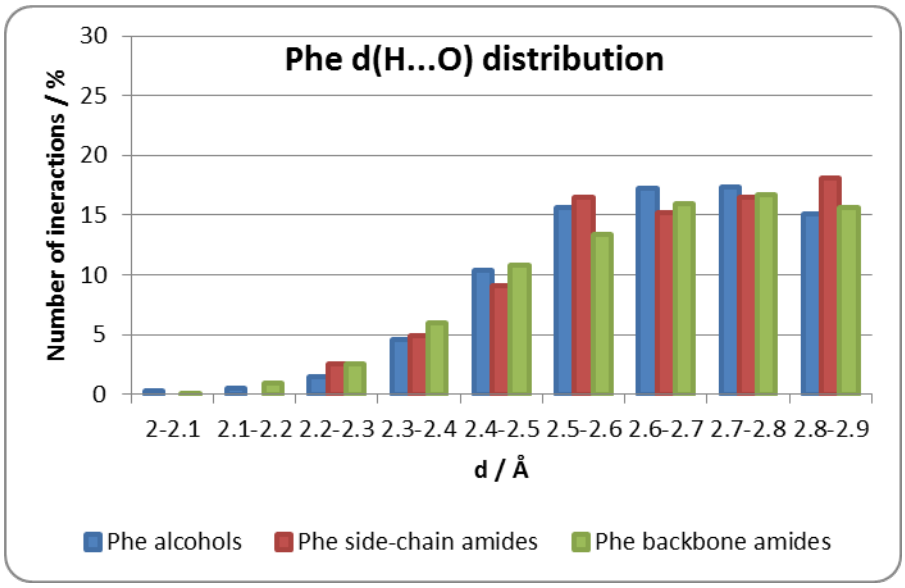
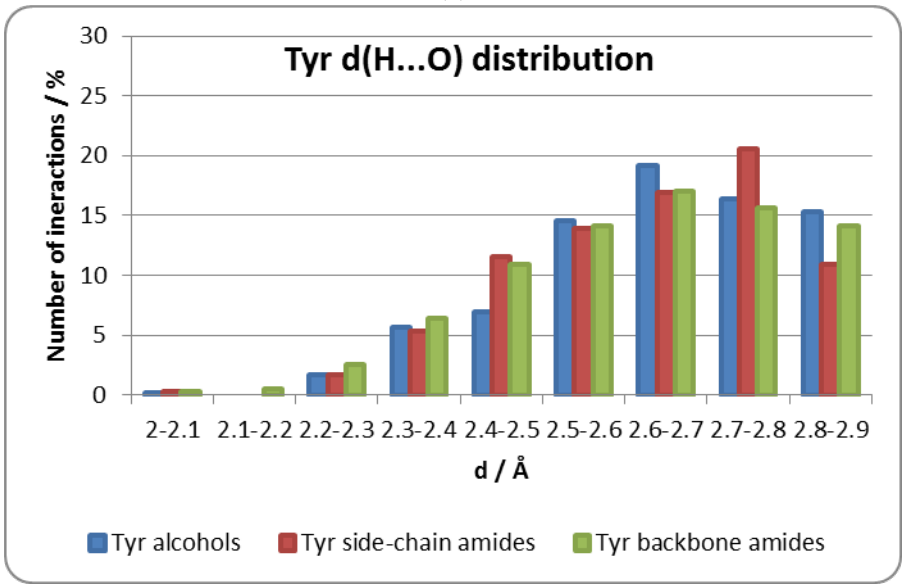
I Distance d(H···O) distributions



(a)



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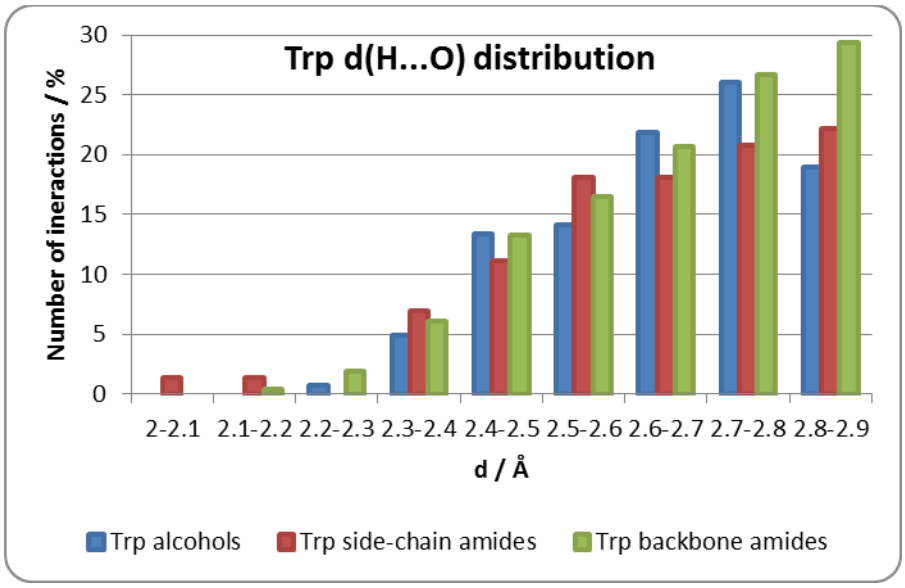
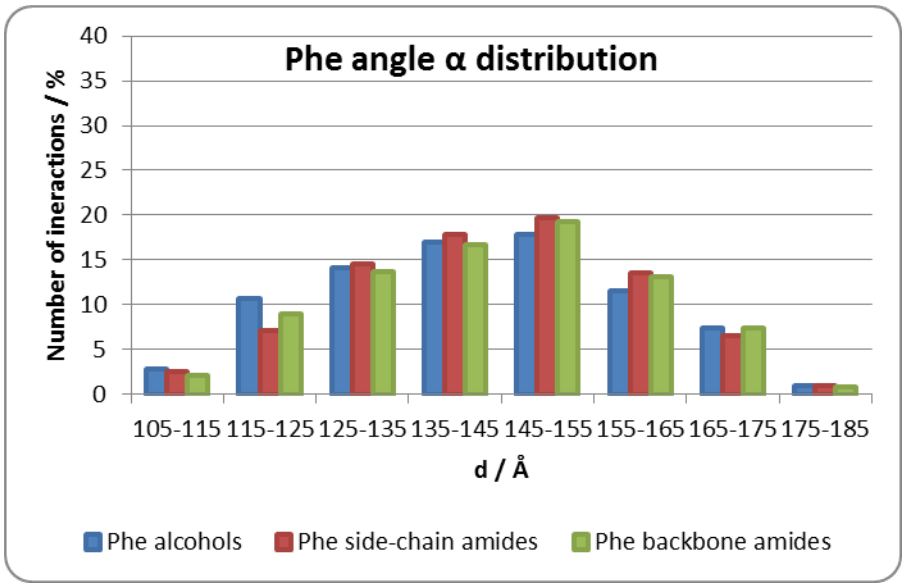


(c)

Figure S1. The total distributions of the distance between the donor hydrogen and the acceptor oxygen, with and without classical hydrogen bonds for the three donors: (a) phenylalanine, (b) tyrosine and (c) tryptophan. The acceptors are represented in different colours: blue for the alcohol group, red for the side-chain amide group and green for the backbone amide group.

II Noncorrected angle α distributions



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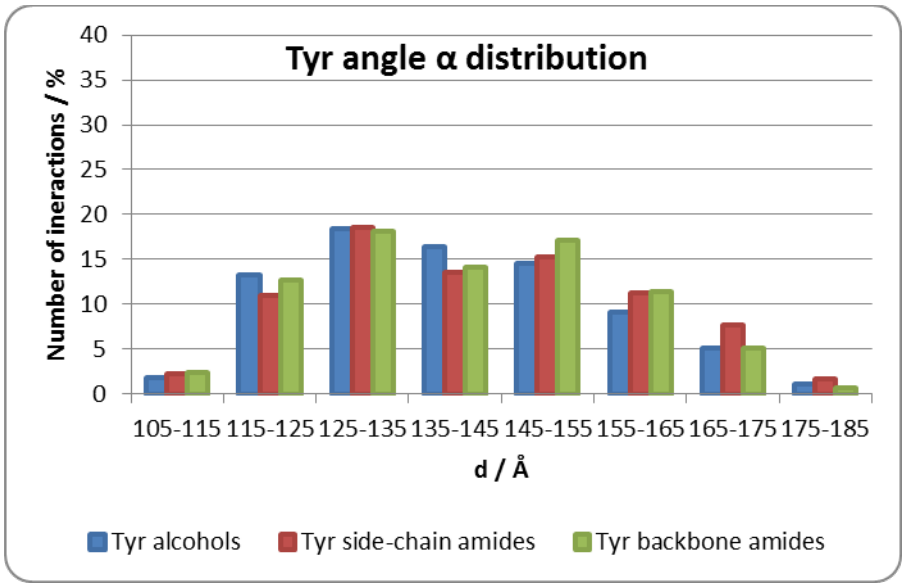

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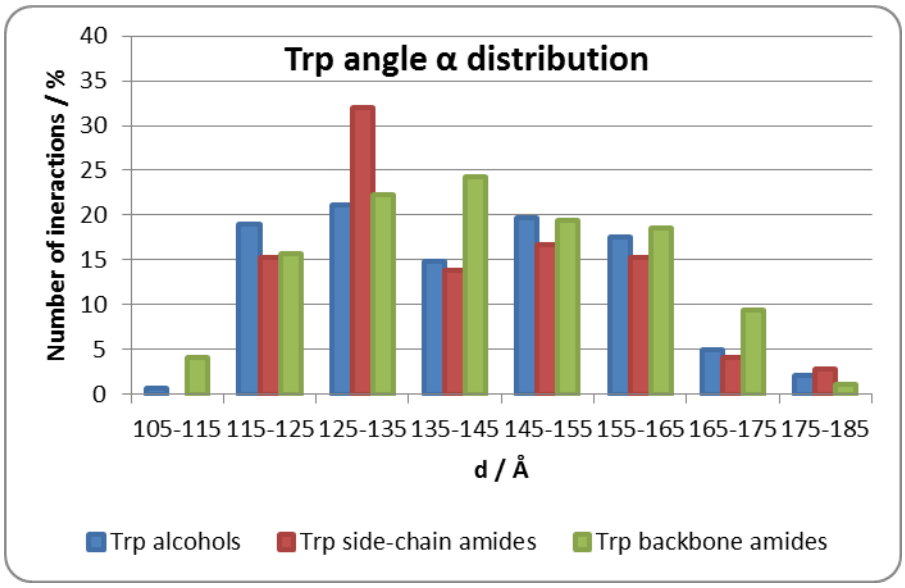
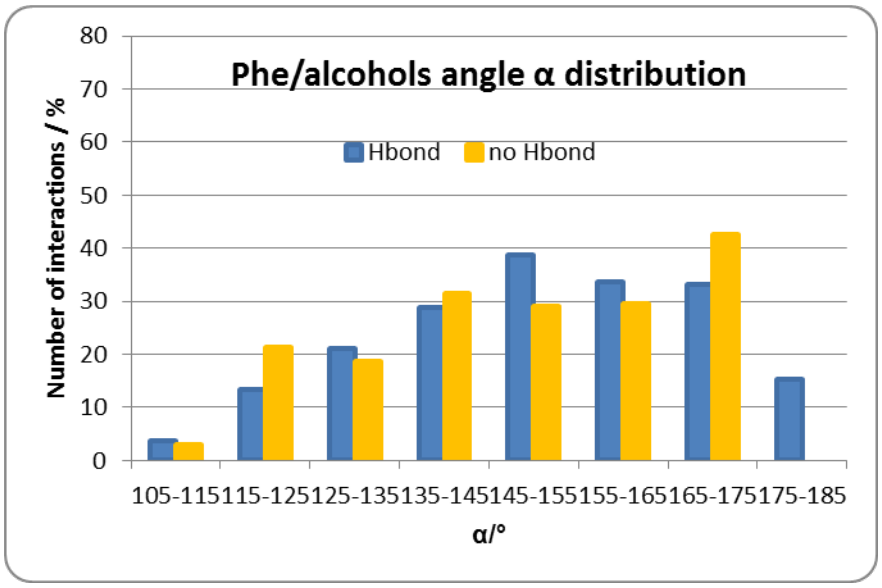


(c)

Figure S2. The noncorrected total angle α distributions, with and without classical hydrogen bonds for the three donors: (a) phenylalanine, (b) tyrosine and (c) tryptophan. The acceptors are represented in different colours: blue for the alcohol group, red for the side-chain amide group and green for the backbone amide group.

III C-H/O angle α distributions with and without classical hydrogen bond



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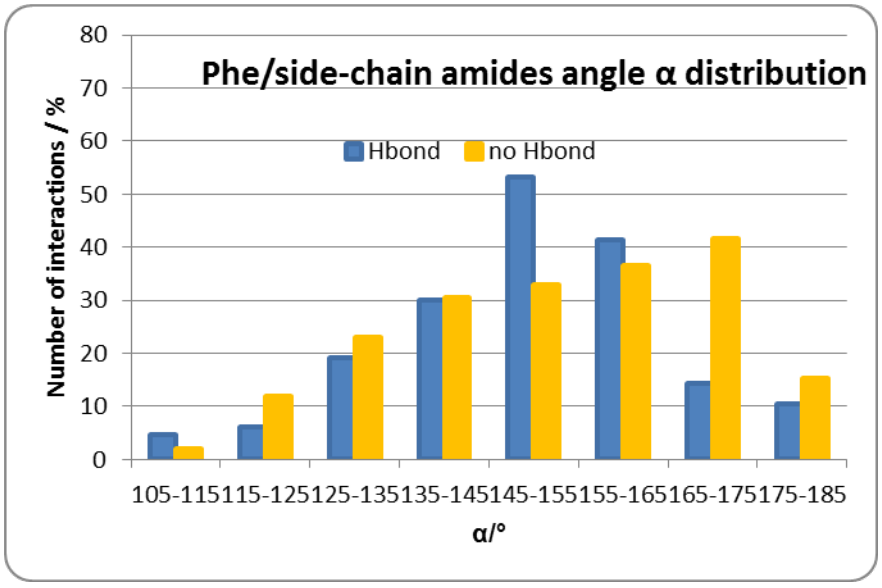

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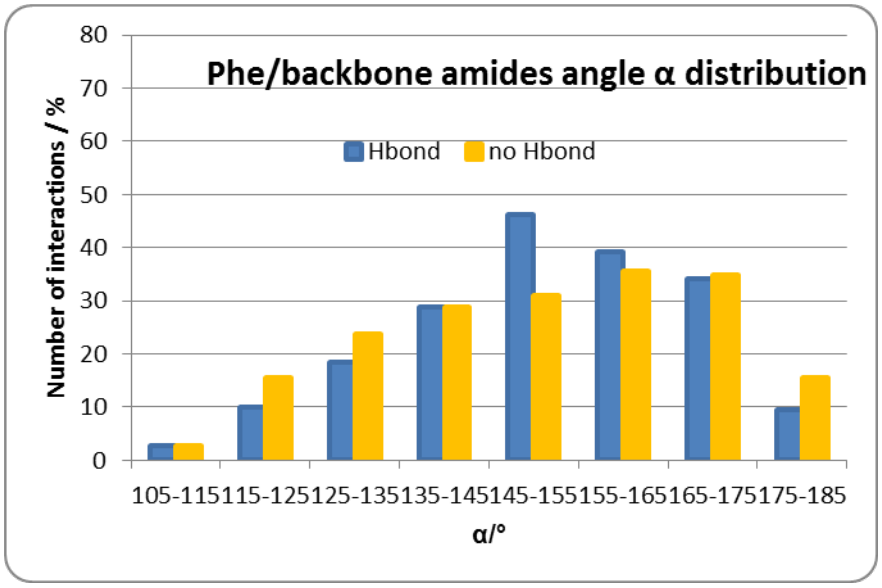
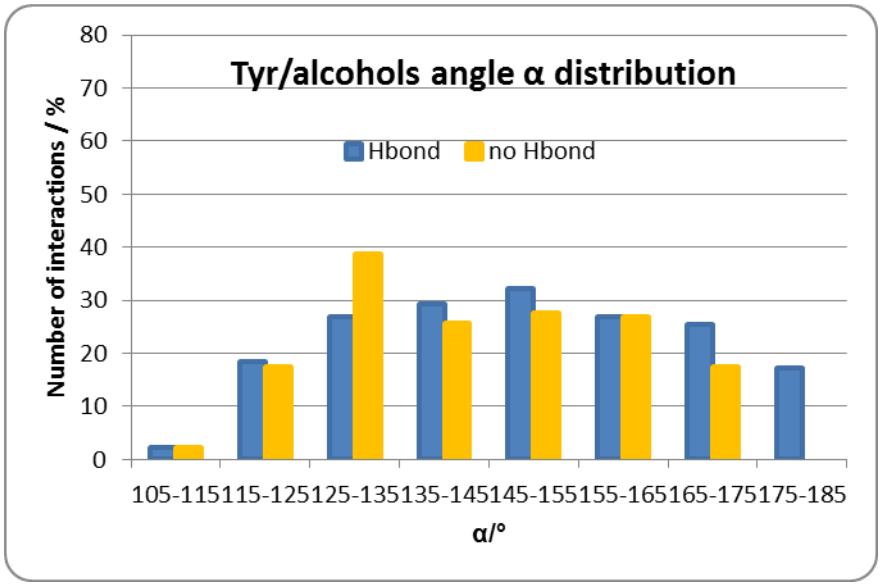


(c)

Figure S3. Corrected angle α distributions for C-H/O interactions with (blue) and without (yellow) simultaneous classical hydrogen bonds for phenylalanine with different acceptors: (a) alcohol group, (b) side-chain amide group and (c) backbone amide group.



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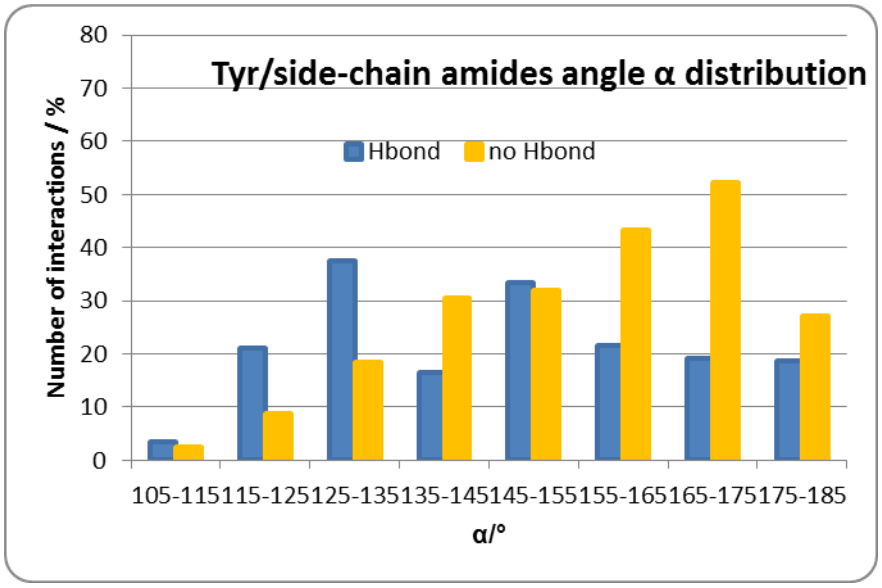

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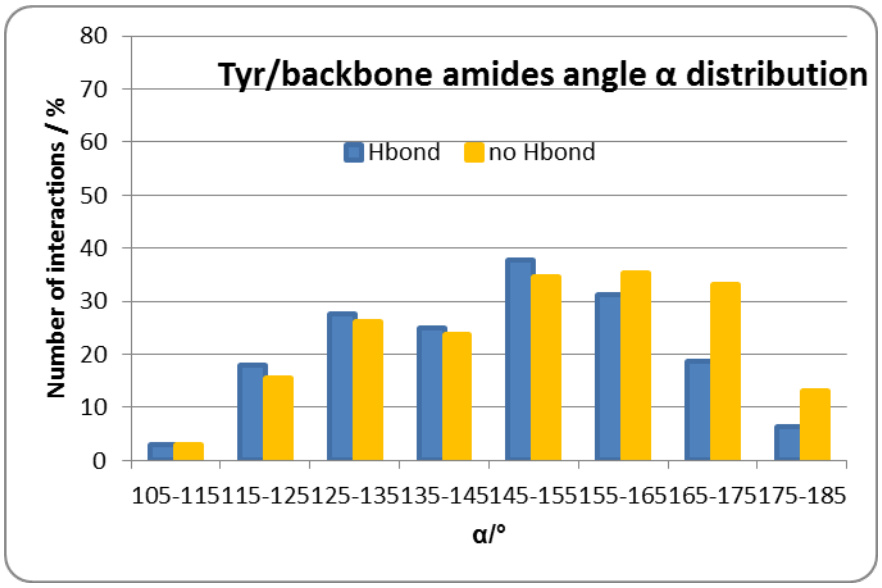
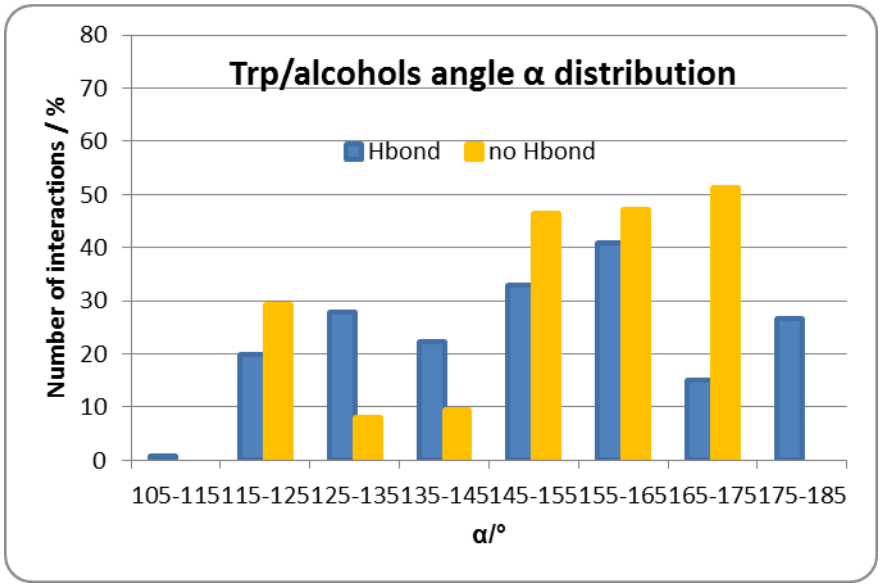
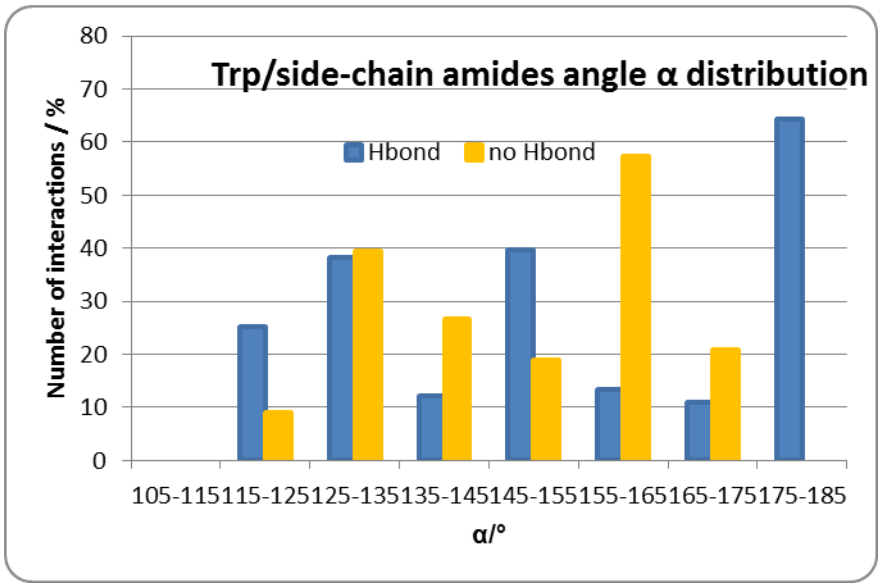


(c)

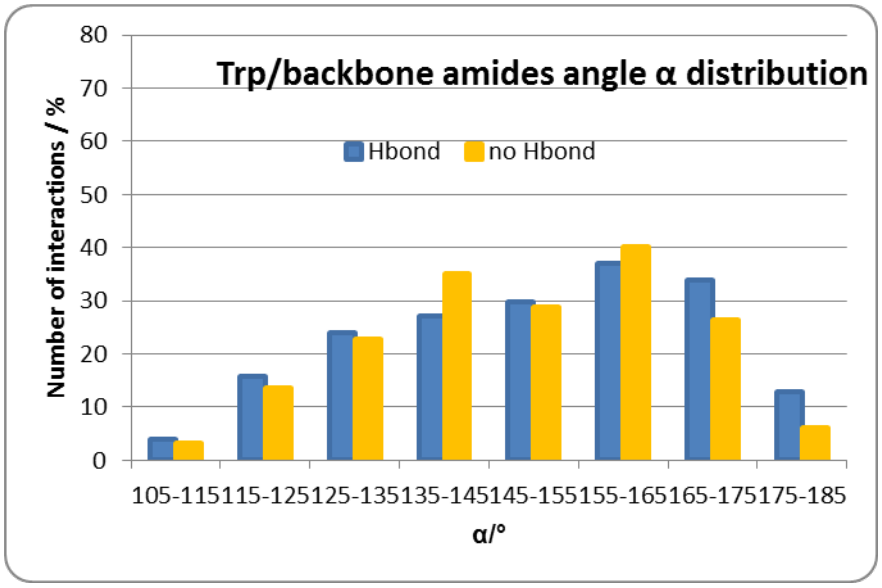
Figure S4. Corrected angle α distributions for C-H/O interactions with (blue) and without (yellow) simultaneous classical hydrogen bonds for tyrosine with different acceptors: (a) alcohol group, (b) side-chain amide group and (c) backbone amide group.


Trp/alcohols angle α distribution
Hbond
no Hbond
Number of interactions / %
0
10
20
30
40
50
60
70
80
105-115
115-125
125-135
135-145
145-155
155-165
165-175
175-185
α/°

(a)


Trp/side-chain amides angle α distribution
Hbond
no Hbond
Number of interactions / %
0
10
20
30
40
50
60
70
80
105-115
115-125
125-135
135-145
145-155
155-165
165-175
175-185
α/°

(b)



(c)

Figure S5. Corrected angle α distributions for C-H/O interactions with (blue) and without (yellow) simultaneous classical hydrogen bonds for tryptophan with different acceptors: (a) alcohol group, (b) side-chain amide group and (c) backbone amide group. The systems tryptophan/alcohol and tryptophan/side-chain amide have small number of interactions making statistics unreliable.

IV C-H/O interaction with simultaneous classical hydrogen bond involving neighboring residue

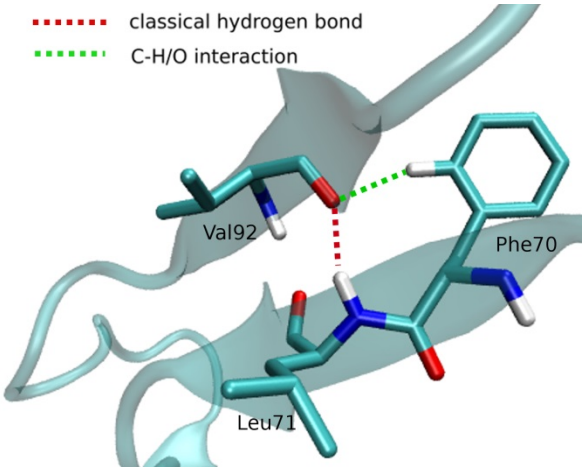


Figure S6. A representative structure of C-H/O interaction with simultaneous classical hydrogen bond between phenylalanine and backbone amide acceptor, involving neighboring residue (Leu71). This is the structure of the runt-related transcription factor 1 (PDB ID 1EAQ).[S1] The C-H/O interaction is in the region around φ=50°; the acceptor oxygen atom (in the amino acid Val92) is positioned at the angle φ=47.34°.

V Number of C-H/O interactions with simultaneous classical hydrogen bonds of the acceptors in all the systems with three acceptors and three donors

Table S1. Number of C-H/O interactions with simultaneous classical hydrogen bonds of the acceptors in all the systems with three acceptors and three donors

Number of H bonds	alcohols		
	acceptors/backbone[a]	acceptors/any atom[b]	%[c]
Phe	23	69	33.3%
Tyr	21	56	37.5%
Trp	2	7	28.6%
Total (3 donors)[d]	46	132	34.8%
Number of H bonds	side-chain amides		
	acceptors/backbone[a]	acceptors/any atom[b]	%[c]
Phe	19	23	82.6%
Tyr	10	13	76.9%
Trp	1	1	100.0%
Total (3 donors)[d]	30	37	81.1%
Number of H bonds	backbone amide		
	acceptors/backbone[a]	acceptors/any atom[b]	%[c]
Phe	677	756	89.6%
Tyr	559	616	90.7%
Trp	119	129	92.2%
Total (3 donors)[d]	1355	1501	90.3%

[a] number of interactions with simultaneous classical hydrogen bonds between the acceptors and a backbone of donors or neighbouring amino acids; [b] number of interactions with simultaneous classical hydrogen bonds between the acceptors and any atom; [c] a fraction of number of interactions with simultaneous classical hydrogen bonds between the acceptors and a backbone of donors or neighbouring amino acids and number of interactions with simultaneous classical hydrogen bonds between the acceptors and any atom, expressed in percentage; [d] the overall acceptors tendencies as it is the sum over the donors.

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(S1) Bäckström, S.; Wolf-Watz, M.; Grundström, C.; Härd, T.; Grundström, T.; Sauer, U. H. *J. Mol. Biol.* **2002**, *322*, 259–272.