Supplementary Material

Table S1. PDB codes and some experimental parameters (chain length, resolution, R-factor) of the protein chains of the datasets Data2.2 (a) and Data1.6 (b).

Excel file TableS1.xls

Table S2. List of PDB codes of Data2.2 (a) and Data1.6 (b).

Excel file TableS2.xls

Table S3. Populations of the (φ,ψ) boxes containing at least 1000 residues in the dataset Data2.2. For each box, the number of residues in α-helix (H), 3(10)-helix (G), β-sheet (E), and polyproline II (P)) is also indicated. The total number of residues in Data2.2 is 1,089,468 (265,543 in E; 13,297 in P; 42,006 in G; 376,101 in H).

BOX	tot	E	P	G	H
1A	2,218	1,150			
2A	6,348	3,550			
3A	5,842	3,197			
4A	5,010	2,478	1		
5A	2,903	921	34		
6A	3,019	529	129		
7A	6,009	534	376	1	
8A	3,939	219	393	3	4
1B	2,025	1,179			
2B	11,185	7,597			
3B	16,369	11,450			
4B	16,989	11,318	3		
5B	9,086	4,856	129		
6B	6,545	2,215	363		1
7B	11,205	1,979	1,062	6	1
8B	17,984	1,647	2,097	33	9
9B	2,421	147	301	12	6
2C	6,144	4,216			
3C	14,815	11,667			

4C	22,848	18,478			
5C	17,728	13,685	136		
6C	12,066	7,707	401		
7C	13,619	5,711	880	5	
8C	26,372	5,590	2,359	37	2
9C	12,919	1,327	1,077	89	12
2D	2,340	1,381			
3D	8,739	6,842			
4D	24,673	21,355	3		
5D	27,966	23,978	127		1
6D	19,972	15,234	418	2	2
7D	15,980	8,848	691	4	
8D	16,345	4,770	1,029	57	1
9D	10,044	936	552	150	3
3E	2,814	1,736			
4E	8,639	6,689			1
5E	13,200	10,223	84		
6E	12,101	8,147	196		2
7E	8,618	4,300	249	2	
8E	2,771	751	100	10	1
3F	1,195	501			
4F	2,602	1,288			
5F	3,678	1,920	5		
6F	3,744	1,844	11		
7F	3,110	1,155	10		2
4G	1,858	394		1	
6G	1,129	257			
7G	2,246	296			1
4H	1,726	128		9	
7H	2,480	93		2	
16I	4,125	333		46	43
4J	1,256	42		116	12
5J	1,010	33		69	

16J	5,725	188	291	29
17J	2,851	115	34	16
4K	2,204	41	282	68
5K	4,524	66	659	37
6K	3,355	39	378	6
16K	1,220	15	188	1
17K	4,884	56	221	13
18K	2,234	21	21	1
4L	2,311	82	140	303
5L	6,632	142	1,251	578
6L	12,812	144	2,133	555
7L	6,282	62	987	94
17L	2,453	15	144	2
18L	4,666	45	94	7
19L	1,796	16	17	
4M	2,047	208	4	562
5M	5,003	526	302	1,258
6M	10,799	299	1,965	2,079
7M	18,634	173	3,446	2,744
8M	12,067	77	4,495	1,090
18M	2,860	26	31	
19M	2,455	21	26	
4N	1,196	110		317
5N	3,488	552	4	1,069
6N	5,704	619	105	1,994
7N	13,278	414	868	5,522
8N	44,922	208	9,870	19,811
9N	9,033	30	3,431	2,204
5O	1,696	295		310
6O	3,671	732		1,236
7O	11,043	732	19	7,171
8O	183,473	506	1,692	172,636
9O	63,823	113	6,009	51,149

5P	1,058	221		80
6P	1,785	452		454
7P	3,595	388		2,004
8P	55,328	212	30	52,919
9P	47,610	78	749	45,021
2X	1,643	814		
3X	1,356	606		
4X	1,057	342		
6X	1,252	114		
7X	1,898	79		

Table S4. Populations (a) and propensity scales (b) of the 95 (φ,ψ) boxes containing at least 1000 residues in the dataset Data2.2.

Excel file TableS4.xls

Table S5. Average (φ,ψ) values at the seven positions of π-helices of the dataset by Karplus PA and colleagues [29].

Position	φ (°)	ψ (°)
PI1	-64.2	-41.0
PI2	-63.3	-47.6
PI3	-71.5	-37.9
PI4	-91.5	-34.5
PI5	-110.5	-52.9
PI6	-69.4	-44.9
PI7	-64.9	-38.4

Table S6. Pair-wise comparison of the propensity scales for the secondary structure elements (α-helix (H), 3(10)-helix (G), β-sheet (E), and polypropline II (P)).The correlation coefficients R and the *p*-values are reported on the right and left side of the diagonal, respectively. The 18AA ensemble is considered.

	E	**G**	**H**	**P**
E		-0.73	-0.27	-0.23
G	<0.001		0.12	-0.05
H	0.28	0.65		0.59
P	0.36	0.83	0.01	

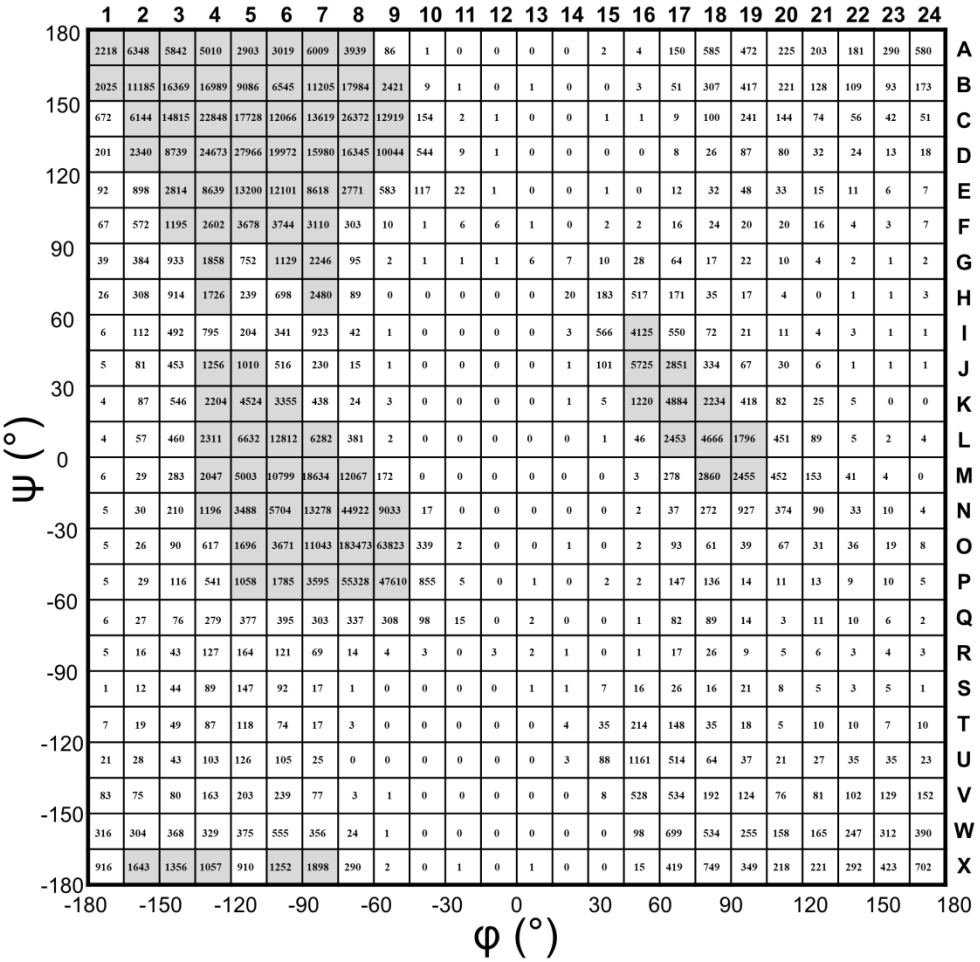


Figure S1. Populations (number of amino acid residues) of the 576 (φ,ψ) boxes of the Ramachandran plot in the dataset Data2.2. Boxes containing at least 1000 residues are colored in light grey. Although with a population >1000 residues, the 16U box has not been included in the study being an isolated box in the Ramachandran space.

Residue	box 1A	Data2.2	Propensity
A	203	91,777	1.086
V	1	81,244	0.006
L	27	106,443	0.125
I	2	66,707	0.015
M	21	18,785	0.549
K	43	56,584	0.373
R	77	54,936	0.688
Q	44	40,054	0.540
E	45	66,055	0.335
H	86	25,918	1.630
S	325	63,476	2.515
T	38	61,329	0.304
W	38	17,806	1.048
Y	105	43,721	1.180
N	122	46,277	1.295
D	128	61,317	1.025
C	71	14,364	2.428
F	133	48,764	1.340
G	709	75,312	4.624
P	0	48,599	0.000
TOTAL	2,218	1,089,468	

Example of calculation of the Chou-Fasman-like propensity of the Leucine (L) residue for the (φ,ψ) box 1A, $P_{1A,L}$:

Number of Leucine residues in the box 1A

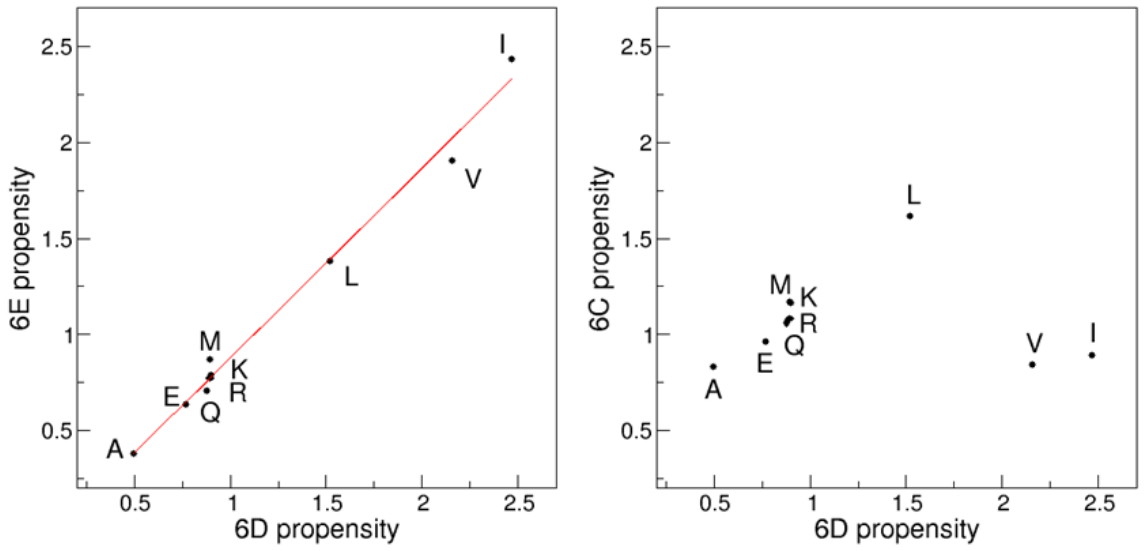
Number of the 20 aminoacid residues in the box 1A

$$P_{1A,L} = \left(\frac{N_{1A,L}}{N_{Data2.2,L}}\right) \Big/ \left(\frac{\sum_{i=1}^{20} N_{1A,i}}{\sum_{i=1}^{20} N_{Data2.2,i}}\right) = \left(\frac{27}{106{,}443}\right) \Big/ \left(\frac{2{,}218}{1{,}089{,}468}\right) = 0.125$$

Number of Leucine residues in the dataset Data2.2

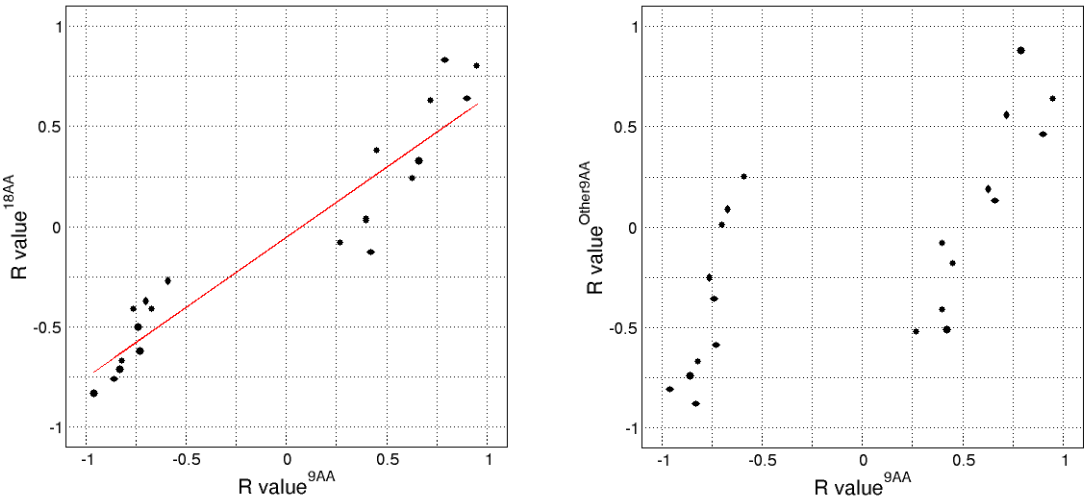
Number of the 20 aminoacid residues in the dataset Data2.2

Figure S2. Example of calculation of the Chou-Fasman-like propensity (see definition (2) in the Methods section) of a certain residue (i.e. Leucine) for a specific box (i.e. box 1A) of the Ramachandran plot.



(a) **(b)**

Figure S3. Comparison of the propensity scales of the 9AA for the couples of boxes (a) 6D-6E and (b) 6D-6C. For the 6D-6E pair the linear regression analysis yielded a correlation coefficient R= 0.995 (p-value<10^{-5}).



(a) **(b)**

Figure S4. Correlation between the R values obtained for the same pair-wise comparison using (a) the 18AA and 9AA amino acid residue ensembles (R= 0.94, $p<10^{-5}$) and (b) the 9AA and Other9AA ensembles.

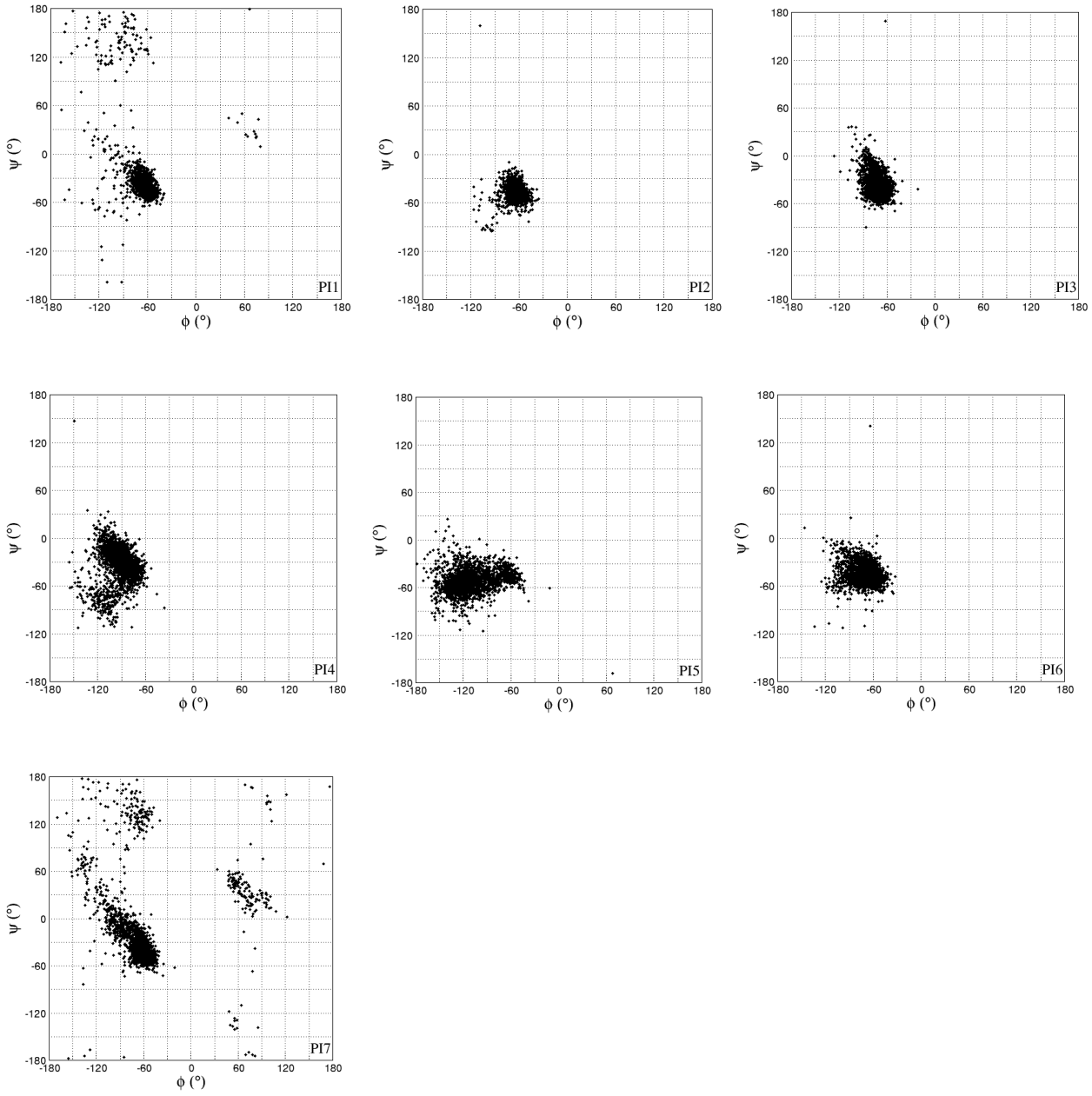
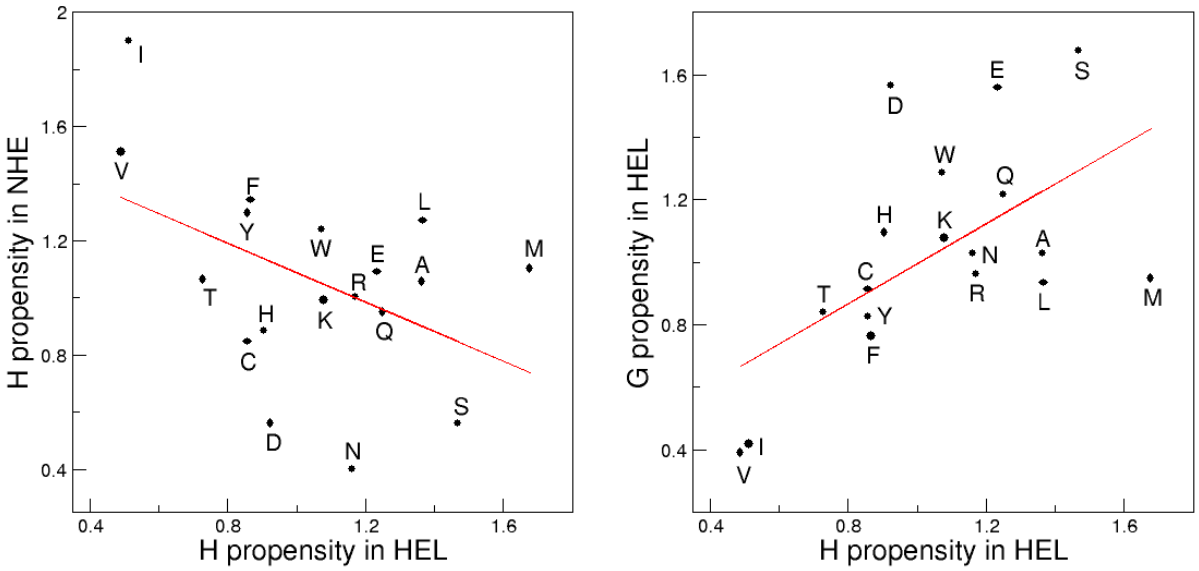


Figure S5. Ramachandran plots showing the conformation adopted by amino acid residues located at the seven positions of π-helices (PI1-PI7).



(a) **(b)**

Figure S6. Significant correlations/anticorrelations of the propensity scales detected in the 18AA ensemble: (**a**) HEL_H *versus* NHE_H (R = -0.46, p=0.055), (**b**) HEL_H *versus* HEL_G (R = 0.59, p=0.010).

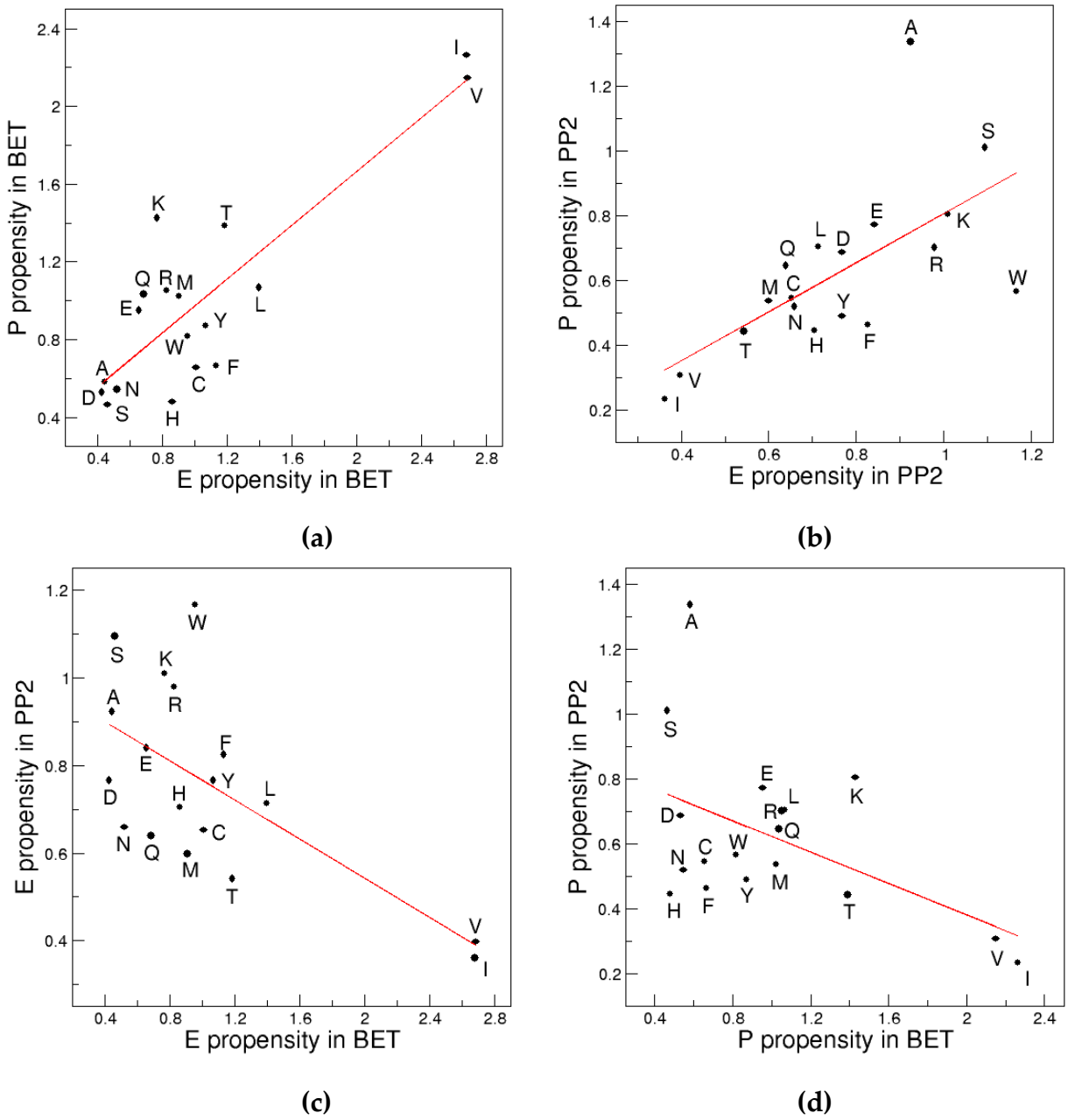
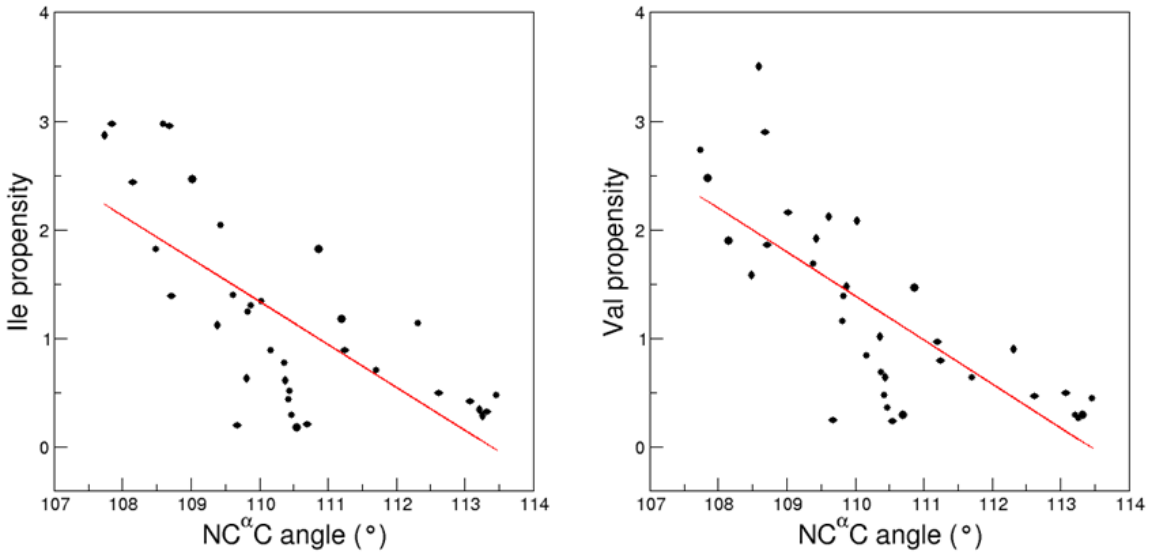


Figure S7. Significant correlations/anticorrelations of the propensity scales detected in the 18AA ensemble: (**a**) BET_E *versus* BET_P (R= 0.87, $p<10^{-5}$), (**b**) PP2_E *versus* PP2_P (R= 0.66, p=0.0029), (**c**) BET_E *versus* PP2_E (R= -0.66, p=0.0029), and (**d**) BET_P *versus* PP2_P (R= -0.49, p=0.039).



(a) **(b)**

Figure S8. Propensities of (**a**) Ile and (**b**) Val residues as a function of the average value of the backbone bond angle τ (NC$^{\alpha}$C) of the (φ, ψ) boxes. Significant anticorrelations have been detected for both Ile (R= -0.72, $p<10^{-5}$) and Val (R= -0.76, $p<10^{-5}$) residues. Amino acid residue propensities and NC$^{\alpha}$C values are calculated in the datasets Data2.2 and Data1.6, respectively.