Supporting Information

Title: Thermodynamics of α- and β-Structure Formation in Proteins.
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Bond lengths (in Å)

------ BACKBONE -------		
N,CA	1.46	
CA,C	1.52	
C,N	1.33	
CA,CB	1.53	
C,O	1.23	
N,H	0.98	
CA,HA	1.08	
CA,2HA	1.08	only GLY
--------- VAL ---------		
CB,CGX	1.52	X=1,2
--------- LEU ---------		
CB,CG	1.53	
CG,CDX	1.52	X=1,2
--------- ILE ---------		
CB,CG1	1.53	
CB,CG2	1.53	
CG1,CD1	1.52	
--------- SER ---------		
CB,OG	1.42	
--------- THR ---------		
CB,OG1	1.43	
CB,CG2	1.52	
--------- CYS ---------		
CB,SD	1.81	
--------- MET ---------		
CB,CG	1.52	
CG,SD	1.81	
SD,CE	1.79	
--------- PRO ---------		
CB,CG	1.51	
CG,CD	1.51	
--------- ASP ---------		
CB,CG	1.52	
CG,ODX	1.25	X=1,2
--------- ASN ---------		
CB,CG	1.52	
CG,OD1	1.23	
CG,ND2	1.33	
--------- GLU ---------		
CB,CG	1.52	
CG,CD	1.52	
CD,OEX	1.25	X=1,2
--------- GLN ---------		
CB,CG	1.52	
CG,CD	1.52	
CD,OE1	1.23	
CG,NE2	1.33	
--------- LYS ---------		
CB,CG	1.52	
CG,CD	1.52	
CD,CE	1.52	
CE,NZ	1.49	
--------- ARG ---------		
CB,CG	1.52	
CG,CD	1.52	
CD,NE	1.46	
NE,CZ	1.33	
CZ,NHX	1.33	X=1,2
--------- HIS ---------		
CB,CG	1.52	
CG,ND1	1.35	*)
--------- PHE ---------		
CB,CG	1.52	
CG,CD1	1.39	*)
--------- TYR ---------		
CB,CG	1.51	
CG,CD1	1.39	*)
CZ,OH	1.38	
--------- TRP ---------		
CB,CG	1.50	
CG,CD1	1.39	*)

All bonds between an H and a side-chain atom have length 1.00 Å.

*) Rings are regular pentagons/hexagons.

Bond angles (in degrees)

------ BACKBONE -------		
N,CA,C	111.0	
CA,C,N	116.6	
C,N,CA	121.7	
N,CA,CB	110.0	
CA,C,O	121.7	
C,N,H	119.2	
N,CA,HA	109.0	
N,CA,2HA	109.0	only GLY
--------- ALA ---------		
CA,CB,XHB	109.5	X=1,2,3
--------- VAL ---------		
CA,CB,CGX	110.7	X=1,2
CA,CB,HB	109.1	
CB,CGY,XHGY	109.5	X=1,2,3; Y=1,2
--------- LEU ---------		
CA,CB,CG	117.1	
CB,CG,CDX	110.1	X=1,2
CA,CB,XHB	107.0	X=1,2
CB,CG,HG	109.3	
CG,CDY,XHDY	109.5	X=1,2,3; Y=1,2
--------- ILE ---------		
CA,CB,CG1	110.4	
CA,CB,CG2	110.4	
CB,CG1,CD1	113.6	
CA,CB,HB	109.2	
CB,CG1,XHG1	108.1	X=1,2
CB,CG2,XHG2	109.5	X=1,2,3
CG1,CD1,XHD1	109.5	X=1,2,3
--------- SER ---------		
CA,CB,OG	110.6	
CA,CB,XHB	109.1	X=1,2
CB,OG,HG	108.0	
--------- THR ---------		
CA,CB,OG1	108.6	
CA,CB,CG2	111.5	
CA,CB,HB	109.3	
CB,OG1,HG1	108.0	
CB,CG2,XHG2	109.5	X=1,2,3
--------- CYS ---------		
CA,CB,SG	113.4	
CA,CB,XHB	108.1	X=1,2
CB,SG,HG	108.0	
--------- MET ---------		
CA,CB,CG	113.5	
CB,CG,SD	111.9	
CG,SD,CE	100.5	
CA,CB,XHB	108.1	X=1,2
CB,CG,XHG	108.7	X=1,2
SD,CE,XHE	109.5	X=1,2,3
--------- PRO ---------		
CA,CB,CG	103.3	
CB,CG,CD	110.8	
CA,CB,XHB	111.6	X=1,2
CB,CG,XHG	109.0	X=1,2
CG,CD,XHD	110.7	X=1,2
--------- ASP ---------		
CA,CB,CG	113.2	
CB,CG,ODX	118.6	X=1,2
CA,CB,XHB	108.2	X=1,2
--------- ASN ---------		
CA,CB,CG	112.6	
CB,CG,OD1	120.9	
CB,CG,ND2	117.0	
CA,CB,XHB	108.4	X=1,2
CG,ND2,XHD2	120.0	X=1,2
--------- GLU ---------		
CA,CB,CG	114.1	
CB,CG,CD	113.2	
CG,CD,OEX	118.5	X=1,2
CA,CB,XHB	108.0	X=1,2
CB,CG,XHG	108.2	X=1,2
--------- GLN ---------		
CA,CB,CG	113.7	
CB,CG,CD	112.6	
CG,CD,OE1	121.0	
CG,CD,NE2	116.9	
CA,CB,XHB	108.1	X=1,2
CB,CG,XHG	108.4	X=1,2
CD,NE2,XHE2	120.0	X=1,2

Bond angles cont.

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--------- LYS ---------
CA,CB,CG          113.8
CB,CG,CD          111.6
CG,CD,CE          111.6
CD,CE,NZ          111.6
CA,CB,XHB         108.1  X=1,2
CB,CG,XHG         108.8  X=1,2
CG,CD,XHD         108.8  X=1,2
CD,CE,XHE         108.8  X=1,2
CE,NZ,XHZ         109.5  X=1,2,3
--------- ARG ---------
CA,CB,CG          113.7
CB,CG,CD          111.5
CG,CD,NE          111.5
CD,NE,CZ          124.4
NE,CZ,NHX         120.0  X=1,2
CA,CB,XHB         108.1  X=1,2
CB,CG,XHG         108.8  X=1,2
CG,CD,XHD         108.8  X=1,2
CZ,NE,HE          120.0
CZ,NHY,XHHY       120.0  X=1,2; Y=1,2
--------- HIS ---------
CA,CB,CG          113.2
CB,CG,ND1         126.0
CA,CB,XHB         108.2  X=1,2
--------- PHE ---------
CA,CB,CG          113.7
CB,CG,CD1         120.0
CA,CB,XHB         108.1  X=1,2
--------- TYR ---------
CA,CB,CG          113.6
CB,CG,CD1         120.0
CE1,CZ,OH         120.0
CA,CB,XHB         108.1  X=1,2
CZ,OH,HH          108.0
--------- TRP ---------
CA,CB,CG          113.8
CB,CG,CD1         126.0
CA,CB,XHB         108.1  X=1,2
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The rings of HIS, PHE, TYR and TRP are regular pentagons/hexagons with hydrogens pointing in the radial direction.

Torsion angles (in degrees)

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------ BACKBONE -------
CA,C,N,CA               180.0
C,N,CA,C - C,N,CA,CB     120.9
C,N,CA,C - C,N,CA,HA    -118.7
C,N,CA,C - C,N,CA,2HA    118.7  only GLY
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For side-chain branch points, we assume exact 2-fold or 3-fold torsional symmetry. The rings of PRO, HIS, PHE, TYR and TRP as well as the atom group NE, CZ, NH1 and NH2 of ARG are planar.

Number of side-chain DOFs (χ_i)

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GLY               0
ALA               1
VAL               3
LEU               4
ILE               4
SER               2
THR               3
CYS               2
MET               4
PRO               0
ASP               2
ASN               3
GLU               3
GLN               4
LYS               5
ARG               4
HIS               2
PHE               2
TYR               3
TRP               2
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