Krivov, Shapovalov, and Dunbrack
Supplemental Data
"Improved prediction of protein side-chain conformations with SCWRL4"

Training set (100 proteins)

135l 1a8q 1agy 1bj7 1bk7 1bkr 1bn6 1c44 1c5h 1chd 1edg 1ew4 1eyh 1f32 1g9o 1gqz
1gyv 1h75 1hd5 1i2h 1i2t 1iuk 1jos 1jyh 1k6a 1kf5 1khi 1kng 1kxo 1l6p 1lmi 1ln4
1lpl 1lzl 1mhn 1noa 1o9z 1oa4 1oi7 1omp 1ow1 1p3c 1p7s 1pgs 1ps4 1q42 1q5z 1qad
1qk8 1qwk 1r26 1r62 1r9w 1ryn 1sno 1t2i 1t3y 1tg0 1tsf 1u53 1uai 1uch 1ucs 1ugn
1uj8 1uoy 1wly 1wpa 1x6q 1x91 1xak 1xte 1y9u 1yck 1yp5 1yrw 1z3y 1zd8 1zeq 1zhv
1zpw 1zzk 2a4v 2ahe 2awg 2b29 2b49 2bv9 2erf 2esk 2fi9 2fk9 2fq3 2fr2 2hvm 2igd
2lis 2ovo 3ezm 4pti

Testing set (379 proteins)

1aho 1atz 1b2p 1b8z 1b9w 1bgf 1byi 1c02 1c48 1cei 1dpt 1dq0 1dv7 1dys 1e5m 1e6f
1edq 1elk 1erz 1es5 1es9 1f41 1f60 1f94 1fcq 1fo9 1fpo 1ftr 1fvk 1g61 1g8a 1g8q
1gmu 1go3 1gpp 1gqn 1gs9 1gso 1gvp 1gxn 1h03 1h4a 1h4y 1hcl 1hm5 1hz6 1hz9 1i4j
1igq 1ijq 1ijy 1ilk 1iu8 1j23 1j2a 1j7g 1jb3 1jcd 1jks 1jy2 1k33 1kmt 1kmz 1kn3
1koe 1kpt 1ku8 1kva 1kve 1kyf 1kzq 1l3k 1lbv 1lm5 1ltu 1m5t 1m6j 1md6 1mf7 1mg7
1mix 1mkk 1mml 1mol 1n1j 1n93 1nar 1nm8 1nwa 1nxm 1oai 1oaq 1ogm 1ok7 1p1x 1p6z
1p9h 1pcf 1pdo 1pe9 1pgv 1pm4 1pxz 1qah 1qkd 1r12 1r29 1r77 1r8n 1rfy 1rgx 1rl0
1rwz 1ryl 1rz2 1s7i 1s7k 1sau 1sh8 1smx 1snt 1sqe 1srv 1suu 1swh 1t1j 1tje 1tks
1tp6 1tua 1tuo 1ty0 1tzv 1u07 1u2h 1u5x 1ueb 1uek 1ujn 1ukf 1uln 1ulr 1unp 1usm
1uxz 1uz3 1v05 1v0s 1v6t 1v7q 1v8e 1v8h 1v8i 1vdk 1ve2 1vgt 1vh5 1vjs 1vpi 1w5r
1w7b 1wba 1wd7 1wka 1wko 1wlg 1wlz 1wm3 1wmh 1wqj 1wtj 1wu9 1wvh 1wyc 1wz3 1x1e
1x2i 1x6i 1xdz 1xfk 1xs0 1xxo 1y2t 1y7y 1yac 1yhh 1yn3 1yo3 1ypf 1yt4 1ytl 1yu5
1yw5 1yxy 1yzm 1z0c 1z0p 1zkr 1zo2 1zrs 1zuh 1zv1 1zva 1zvt 1zxt 2a35 2a6w 2a8f
2ahf 2ahn 2b0a 2b0j 2b2f 2bay 2bk8 2bpd 2bvp 2cg7 2cgh 2chc 2ci3 2ciu 2cov 2cwc
2cwk 2cwl 2cwr 2cyg 2d4p 2d68 2d8e 2dpo 2dqw 2dyu 2e01 2e10 2e3z 2e64 2e7a 2e8f
2e8g 2e9y 2ebb 2ebe 2ecr 2egj 2ehg 2epi 2etx 2ex0 2f23 2f5g 2f6l 2fbn 2fbq 2fd5
2fhz 2fjz 2fl4 2flu 2frg 2fvh 2fw7 2g2u 2g30 2g40 2g69 2g7i 2g7o 2gas 2gdq 2gec
2ggv 2giy 2gkg 2gkv 2gom 2gqv 2gxg 2h14 2h2r 2h2z 2h7w 2h7z 2h8e 2h8o 2hc8 2hlr
2hly 2hoq 2hpl 2hww 2hy5 2hzf 2i3f 2i49 2i5d 2i6v 2ibl 2ic6 2ic7 2iia 2ijk 2ip2
2ipr 2iru 2ium 2ixm 2iy9 2iz6 2j2j 2j5y 2j6b 2j71 2j8b 2j9w 2jcp 2nml 2nnu 2npt
2nrr 2nv0 2o0q 2o2k 2o37 2o6s 2o6x 2oeb 2ohw 2oix 2ol7 2osa 2otu 2p1g 2p38 2p4h
2p52 2p5d 2p5k 2p65 2p84 2pbp 2pbq 2pef 2pet 2pge 2pkf 2pmr 2pnd 2pst 2ptv 2pv2
2pz4 2q8o 2qiy 2qol 2qpw 2qr3 2qt4 2r6u 2r77 2r99 2rcz 2rfa 2rik 2rjd 2rk5 2vc8
2yxf 2yyv 2yz1 2z14 2z1e 2z37 2zfy 3bb7 3bn6 3c4s 6xia

SCWRL4 parameters

van der Waals radii
C: 1.68
N: 1.28
O: 1.29
H: 0.49
S: 1.71

Hydrogen bond parameters
B: 35
d0: 2.08
sigmaD: 0.67
alphaMax: 37
betaMax: 49

Residue specific parameters
Rotamer library weight *k*
FRM model temperature
FRM model c_i for each dihedral degree of freedom ("sigmaboost")

Oct-08	Avrg	ARG	ASN	ASP	CYS	GLN	GLU	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
LogCoeff	2.20	2.27	1.80	2.44	**4.07**	1.61	1.85	2.01	2.18	2.25	2.13	1.95	1.71	**0.76**	2.78	2.96	3.24	2.00	1.62
Temperature	1.70	1.23	1.41	1.48	1.69	1.32	**0.94**	1.35	2.03	2.55	1.27	1.77	1.07	2.62	**3.53**	1.11	0.99	1.96	2.20
SigmaBoost_1	1.25	0.87	**0.62**	1.59	1.69	1.55	0.82	1.84	1.23	1.15	1.62	0.97	1.45	0.78	0.65	0.88	1.28	1.48	**2.09**
SigmaBoost_2	1.30	1.62	1.93	0.63		**0.53**	1.57	0.85	0.98	1.48	0.99	1.54	1.35	1.27	**2.98**	0.88	1.48	0.73	
SigmaBoost_3	1.24	1.67				**1.89**	**0.76**				0.96	1.21						0.96	
SigmaBoost_4	1.58	**0.73**									**1.49**								
SB_Avg	1.31	1.22	1.27	1.11	1.69	1.32	1.05	1.35	1.10	1.31	1.27	1.24	1.40	1.02	1.82	0.88	1.38	1.05	2.09