A potential smoothing algorithm accurately predicts transmembrane helix packing

Rohit V. Pappu, Garland R. Marshall and Jay W. Ponder, *Nature Struct. Biol.* **6**, 50–55 (1999).

Tables 1 and 2 were inadvertently omitted from the text of the paper. They are printed below in full. We regret this error and any confusion it may have caused.

Table 1 Comparison of conformational energies and structural parameters for the set of ten lowest energy conformers obtained from a two-body grid search using model built idealized helices

Interhelical vdW Energy (kcal mol^{-1})	Crossing angle Ω	Contact distance *d* (Å)	Helix A rotation angle α	Helix B rotation angle β	Relative shift *s* (Å)	Smallest r.m.s. Cα superposition on NMR structures
-31.84	-52.81	6.58	-2.75	-3.75	0.00	0.74
-31.31	-159.91	7.49	69.54	68.54	0.00	8.28
-30.37	-165.69	7.33	48.54	47.54	0.00	7.96
-30.23	-135.86	6.62	25.22	24.22	0.00	6.00
-29.75	154.84	7.64	19.14	18.14	0.00	10.02
-28.72	144.14	7.38	3.02	79.97	4.47	9.76
-28.19	-144.63	6.97	57.09	56.09	0.00	6.65
-28.04	-124.14	6.30	46.42	45.42	0.00	7.22
-27.25	-50.82	6.83	103.85	67.89	0.68	4.19
-26.97	159.26	7.70	22.86	21.86	0.00	9.84

Table 2 Comparison of the side chains in the helix dimer interface for the three PSS generated low energy conformers of the GpA helix dimer and the NMR structure[1]

Side chain residue	$\Delta(\%_{sasa})$ for consensus NMR structure	$\Delta(\%_{sasa})$ for PSS global minimum using NMR helices	$\Delta(\%_{sasa})$ for PSS global minimum using idealized helices	$\Delta(\%_{sasa})$ for PSS flexible minimum using ideal helices and fexible side chains
Ile 76 A	42.3	23.6	31.1	32.9
Gly 79 A	93.2	86.9	81.3	79.1
Val 80 A	41.1	38.3	31.4	33.9
Ala 82 A	7.4	10.7	12.0	8.5
Gly 83 A	86.1	95.5	99.6	95.9
Val 84 A	27.6	27.7	25.9	29.8
Thr 87 A	61.5	58.3	56.9	57.8
Ile 91 A	22.1	16.9	11.3	15.3
Leu 75 B	43.1	44.9	37.4	15.2
Ile 76 B	40.6	16.5	31.1	34.5
Gly 79 B	92.9	93.3	81.3	80.3
Val 80 B	42.8	34.8	31.4	34.0
Ala 82 B	8.2	18.3	11.9	8.5
Gly 83 B	87.3	97.5	99.6	95.9
Val 84 B	27.8	25.3	25.9	29.3
Thr 87 B	58.6	58.6	56.9	57.6
Ile 91 B	22.0	14.0	11.3	15.4

[1]Side chains in the interface are characterized using the change in percentage of solvent accessible surface area upon packing. For a given side chain $\Delta(\%_{sasa})$ is defined as the difference in percent solvent accessible surface area of the side chain in the isolated helix monomer and the corresponding percentage for the packed dimer structure. Only side chains with a greater than 10% change in their percentage of accessible surface upon packing are reported. A solvent probe radius of 1.4 Å was used.