

Table S1. Gly-Ala-Gly Peptide

$\Delta E_{vac}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	1.338	4.009	6.779	5.139	4.351
	120	6.322	8.630	9.982	6.019	6.899	6.750
	60	4.576	9.875	4.564	4.462	4.309	3.887
	0	23.484	10.081	10.141	12.923	10.094	12.092
	-60	2.917	1.055	3.800	3.633	4.527	10.844
	-120	0.377	0.147	1.511	0.674	4.872	4.991
$\Delta E_{tot}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	-0.251	1.938	5.542	2.952	3.779
	120	5.845	4.701	6.515	3.884	4.926	5.980
	60	2.016	4.508	0.497	2.660	2.757	1.957
	0	18.156	6.113	8.335	11.312	7.994	7.909
	-60	0.043	-0.789	2.786	1.918	-0.075	5.716
	-120	-0.366	-1.637	-0.550	-1.298	0.840	1.568
$\Delta E_{sol}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	-1.589	-2.070	-1.237	-2.186	-0.572
	120	-0.476	-3.928	-3.467	-2.134	-1.972	-0.770
	60	-2.560	-5.366	-4.067	-1.802	-1.552	-1.929
	0	-5.327	-3.967	-1.806	-1.611	-2.100	-4.183
	-60	-2.873	-1.843	-1.013	-1.715	-4.601	-5.128
	-120	-0.742	-1.784	-2.060	-1.971	-4.031	-3.423

**Table S2.** Gly-Gly-Gly Peptide

$\Delta E_{vac}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	3.109	5.048	5.962	5.048	3.109
	120	1.627	5.524	6.638	2.279	3.384	2.617
	60	3.601	11.032	6.168	4.893	5.152	3.402
	0	22.672	12.491	11.639	13.067	11.639	12.491
	-60	3.601	3.402	5.152	4.893	6.168	11.032
	-120	1.627	2.617	3.384	2.279	6.638	5.524
$\Delta E_{tot}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	2.278	3.500	4.349	3.500	2.278
	120	1.463	2.267	3.612	0.321	2.031	1.844
	60	1.350	6.342	2.253	3.036	4.630	2.345
	0	17.574	9.016	10.319	11.876	10.319	9.016
	-60	1.350	2.345	4.630	3.036	2.253	6.342
	-120	1.463	1.844	2.031	0.321	3.612	2.267
$\Delta E_{sol}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	-0.831	-1.549	-1.613	-1.549	-0.831
	120	-0.165	-3.257	-3.027	-1.958	-1.352	-0.773
	60	-2.251	-4.690	-3.915	-1.858	-0.523	-1.057
	0	-5.098	-3.475	-1.320	-1.191	-1.320	-3.475
	-60	-2.251	-1.057	-0.523	-1.858	-3.915	-4.690
	-120	-0.165	-0.773	-1.352	-1.958	-3.027	-3.257

**Table S3.** Gly-Pro-Gly Peptide

$\Delta E_{vac}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	- 1.261	- 4.512	1.447	8.802	4.522
	120	33.574	39.441	37.313	29.143	33.642	34.660
	60	- 4.994	- 2.367	- 7.293	- 6.245	- 4.409	- 6.765
	0	1.762	- 12.238	- 10.935	- 8.366	- 11.936	- 7.431
	- 60	- 20.327	- 23.151	- 20.077	- 20.559	- 18.953	- 10.237
	- 120	- 18.229	- 19.405	- 20.055	- 20.614	- 13.137	- 13.132
$\Delta E_{tot}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	- 0.357	- 3.744	2.552	9.153	2.322
	120	30.961	37.358	36.787	31.103	33.794	33.499
	60	- 6.390	- 2.084	- 9.242	- 6.252	- 3.689	- 8.524
	0	- 2.101	- 14.589	- 9.314	- 7.131	- 11.686	- 10.393
	- 60	- 21.538	- 22.671	- 17.909	- 20.640	- 20.884	- 13.051
	- 120	- 18.886	- 18.724	- 18.738	- 19.395	- 13.376	- 15.504
$\Delta E_{sol}$	$\phi$						
$\psi$		$\pm 180$	120	60	0	-60	-120
	$\pm 180$	0.000	0.903	0.767	1.105	0.350	- 2.201
	120	- 2.614	- 2.083	- 0.526	1.960	0.152	- 1.162
	60	- 1.396	0.283	- 1.950	- 0.007	0.719	- 1.759
	0	- 3.863	- 2.352	1.620	1.235	0.250	- 2.963
	- 60	- 1.212	0.479	2.167	- 0.082	- 1.932	- 2.814
	- 120	- 0.658	0.681	1.316	1.219	- 0.240	- 2.373

**Table S4.** Special Points

Peptide	$\alpha$ -helix (-57,-47)	parallel- $\beta$ (-119,113)	antiparallel- $\beta$ (-139,135)
Gly-Ala-Gly			
$\Delta E_{vac}$	2.605	-1.473	-4.078
$\Delta E_{tot}$	0.395	-0.487	-0.882
$\Delta E_{sol}$	-0.663	-0.972	-0.308
Gly-Gly-Gly			
$\Delta E_{vac}$	4.445	1.092	-3.353
$\Delta E_{tot}$	2.912	2.040	-0.872
$\Delta E_{sol}$	0.609	0.583	-0.026
Gly-Pro-Gly			
$\Delta E_{vac}$	-20.947	-22.621	-1.674
$\Delta E_{tot}$	-19.578	-18.588	0.989
$\Delta E_{sol}$	-16.273	-16.473	-0.200