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Supplemental Information

New Dynamic Rotamer Libraries: Data-Driven Analysis of Side-Chain Conformational Propensities

Clare-Louise Towse, Steven J. Rysavy, Ivan M. Vulovic, and Valerie Daggett

Supplemental Data

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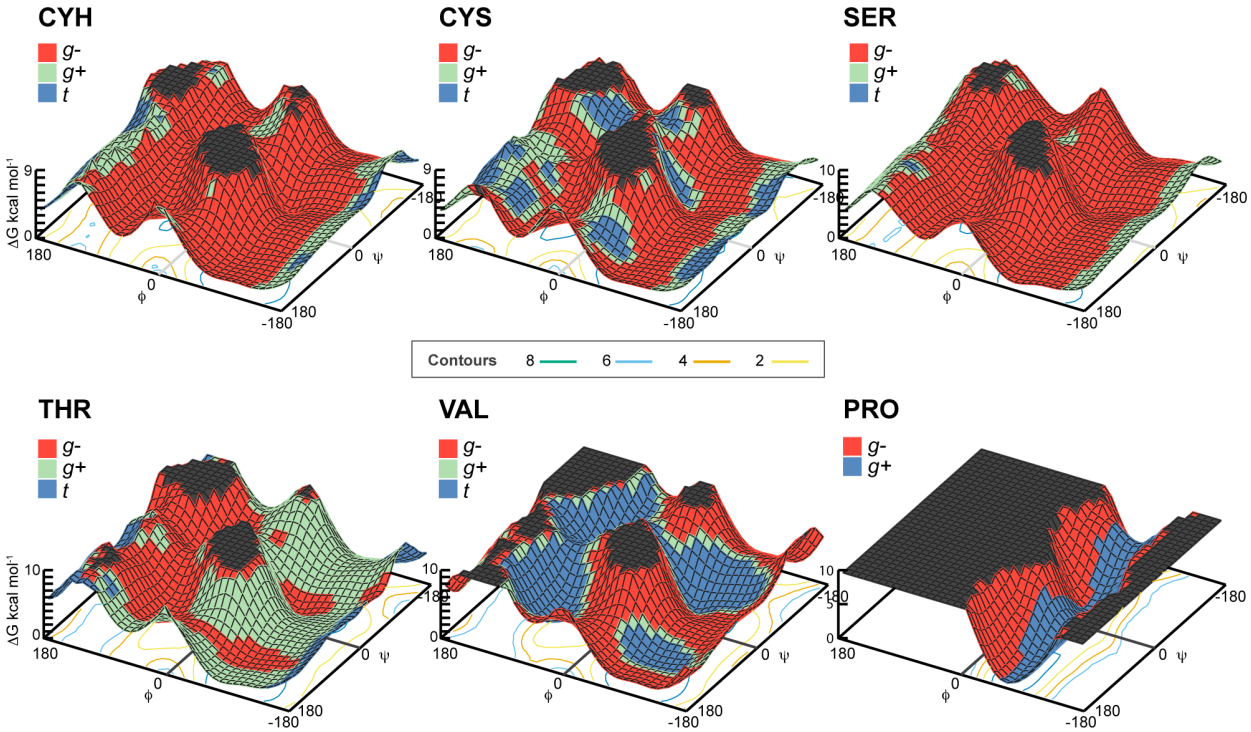
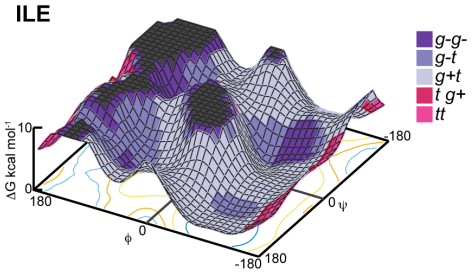


Figure S1: (Related to Figure 6) Rotamer preferences taken from the backbone-dependent (BBDEP) rotamer library for amino acids with only one side chain χ-angle. Free energy landscapes of the ϕ/ψ distributions are shown with the landscapes colored by the preferred rotamer associated with the backbone angles within 5°×5° degree ϕ/ψ bins to illustrate the relationship between rotameric propensities and the relative energies of backbone conformations. Insurmountable energy barriers are shaded black.

Pure Rotameric Side Chains

ILE



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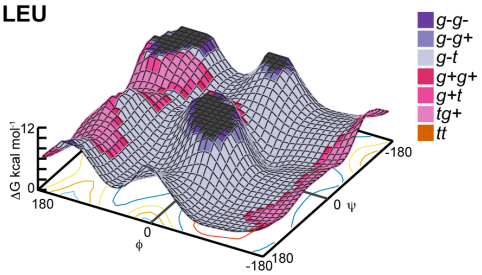

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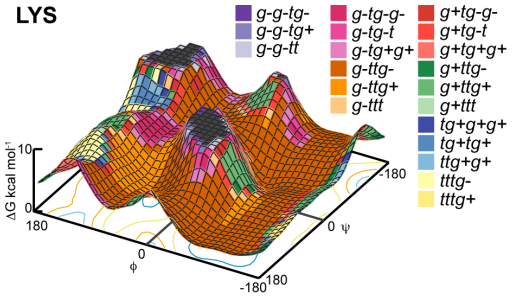
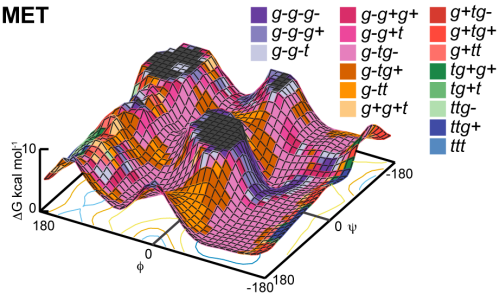
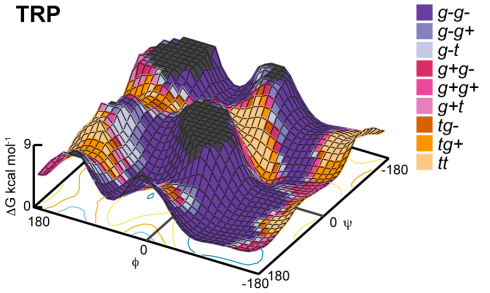


MET

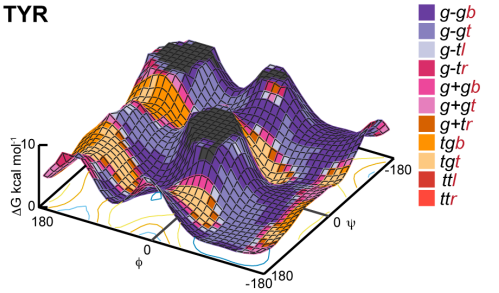


Aromatic Side Chains

TRP

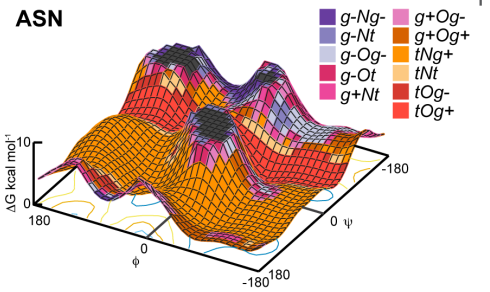


TYR



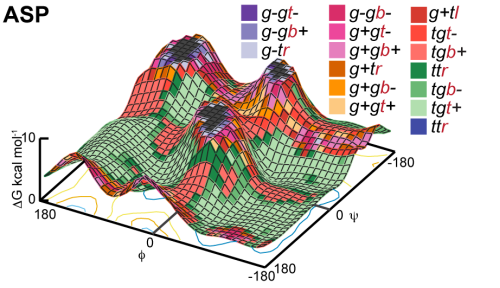
Amide Side Chain

ASN

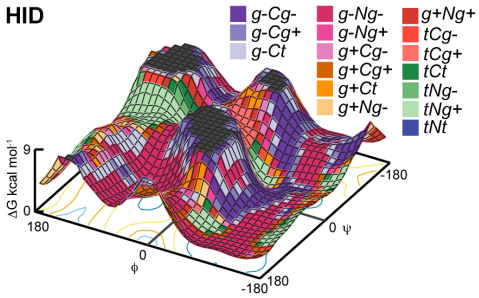


Charged Side Chains

ASP



HID



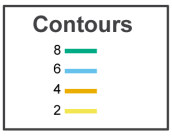


Figure S2: (Related to Figure 6) Rotamer preferences taken from the backbone-dependent (BBDEP) rotamer library for a selection of amino acids with longer side chains and representing different side chain functional groups. Free energy landscapes of the ϕ/ψ distributions are shown with the landscapes colored by the preferred rotamer associated with the backbone angles within 5°×5° degree ϕ/ψ bins to illustrate the relationship between rotameric propensities and the relative energies of backbone conformations. Insurmountable energy barriers are shaded black. Rotamer definitions are as provided in Figure 6, where a residue has split bin definitions, part of the rotamer label is highlighted in red to denote the precise top, bottom, left or right portion of the bin populated.

Table S1: (Related to Figures 5, 8 and 9) Independent (BBIND) and secondary structure region-dependent (RSS) rotamer probabilities. Percentage populations lower than 0.01 are indicated as such to acknowledge that, while substantially smaller populations, rotamer instances were observed in order to delineate from cases where there were no rotamer samples.

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
ARG	g+	g+	g+	g+	0.02%	0.02%	<0.01%	<0.01%	0.03%	<0.01%	<0.01%
ARG	g+	g+	g+	t	0.03%	0.02%	<0.01%	<0.01%	0.03%	0.12%	0.01%
ARG	g+	g+	g+	g-	<0.01%	<0.01%	<0.01%	<0.01%	0.01%	<0.01%	-
ARG	g+	g+	t	g+	0.01%	<0.01%	<0.01%	<0.01%	0.01%	0.06%	<0.01%
ARG	g+	g+	t	t	0.08%	0.01%	0.07%	<0.01%	0.24%	0.18%	0.01%
ARG	g+	g+	t	g-	0.01%	<0.01%	0.08%	-	0.02%	0.02%	<0.01%
ARG	g+	g+	g-	g+	<0.01%	<0.01%	<0.01%	-	<0.01%	-	<0.01%
ARG	g+	g+	g-	t	0.02%	<0.01%	0.17%	0.01%	0.01%	0.01%	<0.01%
ARG	g+	g+	g-	g-	0.01%	<0.01%	0.01%	-	0.01%	0.01%	<0.01%
ARG	g+	t	g+	g+	0.48%	0.10%	0.58%	0.03%	1.17%	0.77%	1.51%
ARG	g+	t	g+	t	0.86%	0.15%	0.98%	0.05%	1.75%	1.72%	1.65%
ARG	g+	t	g+	g-	0.08%	0.01%	0.10%	<0.01%	0.24%	0.12%	0.07%
ARG	g+	t	t	g+	0.68%	0.24%	1.11%	0.01%	1.35%	1.15%	0.45%
ARG	g+	t	t	t	0.64%	0.13%	0.72%	<0.01%	1.86%	1.16%	0.76%
ARG	g+	t	t	g-	0.39%	0.11%	0.25%	0.01%	0.96%	0.81%	0.22%
ARG	g+	t	g-	g+	0.08%	0.03%	0.05%	<0.01%	0.20%	0.18%	0.01%
ARG	g+	t	g-	t	0.70%	0.15%	0.69%	0.02%	1.70%	1.46%	0.71%
ARG	g+	t	g-	g-	0.44%	0.25%	0.40%	0.01%	0.76%	0.87%	0.35%
ARG	g+	g-	g+	g+	0.01%	<0.01%	0.01%	<0.01%	<0.01%	0.01%	<0.01%
ARG	g+	g-	g+	t	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
ARG	g+	g-	g+	g-	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
ARG	g+	g-	t	g+	<0.01%	<0.01%	0.02%	-	<0.01%	<0.01%	<0.01%
ARG	g+	g-	t	t	0.01%	<0.01%	0.02%	<0.01%	0.05%	0.01%	0.04%
ARG	g+	g-	t	g-	0.01%	<0.01%	<0.01%	-	0.03%	0.01%	<0.01%
ARG	g+	g-	g-	g+	<0.01%	<0.01%	<0.01%	-	0.02%	<0.01%	<0.01%
ARG	g+	g-	g-	t	0.02%	<0.01%	0.01%	-	0.03%	0.07%	<0.01%
ARG	g+	g-	g-	g-	<0.01%	<0.01%	<0.01%	-	<0.01%	0.01%	<0.01%
ARG	t	g+	g+	g+	0.31%	0.34%	0.31%	0.18%	0.33%	0.11%	0.36%
ARG	t	g+	g+	t	0.75%	0.89%	1.04%	0.73%	0.65%	0.34%	0.52%
ARG	t	g+	g+	g-	0.05%	0.06%	0.03%	<0.01%	0.06%	0.02%	0.09%
ARG	t	g+	t	g+	0.58%	0.85%	0.64%	0.01%	0.38%	0.18%	0.64%
ARG	t	g+	t	t	1.26%	1.87%	0.86%	0.36%	0.91%	0.44%	0.33%
ARG	t	g+	t	g-	0.47%	0.59%	0.66%	0.18%	0.31%	0.36%	0.20%
ARG	t	g+	g-	g+	0.08%	0.14%	0.01%	<0.01%	0.02%	<0.01%	<0.01%
ARG	t	g+	g-	t	0.11%	0.14%	0.06%	0.12%	0.11%	0.05%	0.04%
ARG	t	g+	g-	g-	0.27%	0.38%	0.60%	0.01%	0.09%	0.08%	0.17%
ARG	t	t	g+	g+	2.75%	4.36%	1.15%	0.27%	1.21%	1.07%	1.18%
ARG	t	t	g+	t	3.37%	4.08%	1.45%	2.18%	3.43%	2.59%	2.49%
ARG	t	t	g+	g-	0.62%	1.06%	0.17%	0.05%	0.23%	0.13%	0.07%
ARG	t	t	t	g+	0.71%	0.70%	0.72%	0.38%	1.05%	0.58%	0.68%
ARG	t	t	t	t	1.92%	1.68%	1.34%	0.95%	3.43%	1.93%	2.36%
ARG	t	t	t	g-	1.05%	1.17%	0.40%	0.17%	1.53%	0.67%	2.23%
ARG	t	t	g-	g+	0.45%	0.71%	0.25%	0.04%	0.21%	0.14%	0.13%
ARG	t	t	g-	t	2.22%	2.65%	2.31%	1.16%	2.49%	0.98%	2.23%
ARG	t	t	g-	g-	1.17%	1.24%	1.29%	0.99%	1.44%	0.82%	0.84%
ARG	t	g-	g+	g+	0.03%	0.02%	0.07%	<0.01%	0.01%	<0.01%	0.41%
ARG	t	g-	g+	t	0.03%	0.03%	0.02%	0.03%	0.04%	0.01%	0.10%
ARG	t	g-	g+	g-	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
ARG	t	g-	t	g+	0.11%	0.12%	0.06%	0.10%	0.11%	0.10%	0.08%
ARG	t	g-	t	t	0.32%	0.28%	0.17%	0.05%	0.62%	0.36%	0.69%
ARG	t	g-	t	g-	0.05%	0.06%	0.08%	<0.01%	0.07%	0.01%	0.11%
ARG	t	g-	g-	g+	0.09%	0.07%	0.02%	0.33%	0.17%	0.04%	0.11%
ARG	t	g-	g-	t	0.41%	0.61%	0.40%	0.09%	0.19%	0.18%	0.09%
ARG	t	g-	g-	g-	0.06%	0.07%	0.05%	0.11%	0.08%	0.02%	0.19%
ARG	g-	g+	g+	g+	0.17%	0.17%	0.39%	0.13%	0.11%	0.22%	0.06%
ARG	g-	g+	g+	t	0.44%	0.48%	0.75%	0.76%	0.33%	0.25%	0.29%
ARG	g-	g+	g+	g-	0.04%	<0.01%	0.01%	0.03%	0.02%	0.02%	0.02%
ARG	g-	g+	t	g+	0.10%	0.04%	0.23%	0.11%	0.18%	0.09%	0.47%
ARG	g-	g+	t	t	0.39%	0.30%	0.70%	0.54%	0.49%	0.45%	0.49%
ARG	g-	g+	t	g-	0.11%	0.08%	0.16%	0.14%	0.18%	0.09%	0.14%
ARG	g-	g+	g-	g+	0.01%	<0.01%	<0.01%	<0.01%	0.01%	0.02%	<0.01%
ARG	g-	g+	g-	t	0.11%	0.19%	0.03%	0.04%	0.04%	0.04%	0.01%
ARG	g-	g+	g-	g-	0.03%	0.03%	0.04%	0.01%	0.02%	0.05%	0.05%
ARG	g-	t	g+	g+	4.67%	4.60%	4.29%	7.68%	4.41%	4.63%	4.24%
ARG	g-	t	g+	t	11.72%	11.58%	11.42%	12.40%	10.64%	13.00%	13.00%
ARG	g-	t	g+	g-	0.75%	0.54%	0.75%	0.82%	0.97%	1.12%	1.44%
ARG	g-	t	t	g+	3.48%	3.01%	3.42%	4.45%	3.89%	4.42%	3.80%
ARG	g-	t	t	t	11.68%	13.08%	9.68%	11.80%	9.63%	10.09%	11.63%
ARG	g-	t	t	g-	4.00%	3.53%	4.12%	4.76%	4.46%	5.15%	3.25%
ARG	g-	t	g-	g+	2.17%	2.70%	2.16%	1.40%	1.28%	1.26%	1.94%
ARG	g-	t	g-	t	10.92%	7.28%	13.41%	21.19%	13.18%	15.14%	15.87%
ARG	g-	t	g-	g-	11.06%	13.61%	9.02%	12.80%	6.36%	8.14%	8.45%
ARG	g-	g-	g+	g+	0.69%	1.00%	0.39%	0.28%	0.32%	0.43%	0.11%
ARG	g-	g-	g+	t	0.83%	0.69%	2.04%	0.37%	0.90%	0.97%	0.82%
ARG	g-	g-	g+	g-	0.13%	0.17%	0.13%	0.11%	0.09%	0.13%	0.03%
ARG	g-	g-	t	g+	1.30%	1.08%	1.57%	1.75%	1.45%	1.52%	1.34%
ARG	g-	g-	t	t	3.76%	3.41%	5.46%	3.38%	3.46%	4.58%	2.67%
ARG	g-	g-	t	g-	2.16%	1.39%	4.65%	1.83%	3.79%	1.73%	3.60%
ARG	g-	g-	g-	g+	0.40%	0.54%	0.20%	0.05%	0.21%	0.32%	0.06%
ARG	g-	g-	g-	t	3.64%	3.87%	3.67%	3.42%	2.64%	4.00%	2.32%
ARG	g-	g-	g-	g-	1.41%	1.23%	1.85%	1.12%	1.32%	2.19%	1.75%
ASN	g+	Ng+			0.15%	0.05%	0.10%	0.01%	0.39%	0.22%	0.11%
ASN	g+	Og-			1.01%	0.22%	0.41%	0.02%	1.97%	3.25%	0.39%
ASN	g+	Nt			0.87%	0.08%	0.23%	<0.01%	1.65%	2.56%	0.34%
ASN	g+	Og+			2.38%	0.33%	1.14%	0.12%	4.00%	8.38%	1.32%
ASN	g+	Ng-			0.25%	0.07%	0.23%	0.02%	0.38%	0.55%	0.40%
ASN	g+	Ot			<0.01%	-	-	-	<0.01%	<0.01%	<0.01%
ASN	t	Ng+			25.68%	16.67%	18.33%	46.06%	35.35%	26.84%	42.35%
ASN	t	Og-			20.39%	16.14%	18.43%	28.71%	24.46%	24.14%	24.29%
ASN	t	Nt			11.18%	15.45%	14.84%	6.76%	6.97%	4.76%	8.96%
ASN	t	Og+			25.14%	39.03%	37.30%	7.15%	12.01%	11.21%	9.14%
ASN	t	Ng-			1.05%	0.95%	1.07%	0.95%	1.38%	1.02%	1.45%
ASN	t	Ot			0.19%	0.17%	0.14%	0.19%	0.29%	0.08%	0.45%
ASN	g-	Ng+			0.62%	0.80%	0.41%	0.26%	0.59%	0.58%	0.39%
ASN	g-	Og-			5.27%	5.26%	3.17%	3.29%	4.72%	7.42%	5.27%
ASN	g-	Nt			2.09%	2.85%	0.82%	0.70%	1.42%	2.98%	0.80%
ASN	g-	Og+			1.85%	1.12%	1.76%	1.93%	2.30%	3.11%	1.94%
ASN	g-	Ng-			1.83%	0.76%	1.54%	3.78%	2.08%	2.86%	2.36%
ASN	g-	Ot			0.05%	0.06%	0.07%	0.04%	0.04%	0.05%	0.04%
ASP	g+	g+			1.40%	0.16%	0.22%	1.16%	3.60%	3.69%	1.61%
ASP	g+	t			0.30%	0.07%	<0.01%	<0.01%	0.84%	0.62%	0.45%
ASP	g+	g-			2.56%	0.32%	0.36%	1.18%	5.48%	7.27%	3.57%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
ASP	t	g+			66.45%	74.31%	75.36%	75.20%	46.99%	39.72%	65.41%
ASP	t	t			7.38%	6.71%	7.48%	5.94%	8.41%	5.35%	11.24%
ASP	t	g-			12.81%	10.23%	10.67%	11.97%	19.14%	22.33%	11.95%
ASP	g-	g+			2.10%	1.62%	1.09%	1.22%	3.97%	6.09%	1.41%
ASP	g-	t			1.48%	1.81%	0.67%	0.40%	1.78%	4.09%	0.33%
ASP	g-	g-			5.51%	4.77%	4.15%	2.92%	9.78%	10.84%	4.02%
CYH	g+				14.00%	2.83%	13.44%	1.69%	25.15%	20.62%	25.15%
CYH	t				16.97%	23.23%	20.05%	13.83%	13.39%	10.25%	17.16%
CYH	g-				69.03%	73.94%	66.51%	84.48%	61.46%	69.13%	57.69%
CYS	g+				13.64%	3.36%	17.44%	3.18%	18.21%	18.80%	15.92%
CYS	t				30.17%	43.79%	29.08%	34.61%	28.03%	17.34%	39.64%
CYS	g-				56.19%	52.85%	53.48%	62.21%	53.76%	63.86%	44.43%
GLN	g+	g+	Ng+		0.01%	<0.01%	0.01%	<0.01%	0.02%	0.03%	0.01%
GLN	g+	g+	Og-		0.01%	<0.01%	<0.01%	<0.01%	0.01%	0.02%	<0.01%
GLN	g+	g+	Nt		<0.01%	<0.01%	<0.01%	-	0.02%	0.02%	<0.01%
GLN	g+	g+	Og+		0.01%	<0.01%	<0.01%	<0.01%	0.04%	0.03%	<0.01%
GLN	g+	g+	Ng-		<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
GLN	g+	g+	Ot		<0.01%	<0.01%	-	-	<0.01%	<0.01%	<0.01%
GLN	g+	t	Ng+		0.52%	0.08%	0.60%	0.02%	1.46%	0.94%	1.39%
GLN	g+	t	Og-		0.51%	0.10%	0.61%	0.02%	1.41%	0.98%	1.27%
GLN	g+	t	Nt		0.29%	0.03%	0.26%	0.02%	0.98%	0.69%	0.66%
GLN	g+	t	Og+		0.58%	0.09%	0.53%	0.03%	1.78%	1.29%	1.10%
GLN	g+	t	Ng-		0.42%	0.06%	0.34%	0.02%	1.29%	1.02%	0.57%
GLN	g+	t	Ot		0.08%	0.01%	0.08%	<0.01%	0.28%	0.18%	0.16%
GLN	g+	g-	Ng+		<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
GLN	g+	g-	Og-		0.01%	<0.01%	<0.01%	<0.01%	0.04%	0.01%	0.01%
GLN	g+	g-	Nt		0.01%	<0.01%	<0.01%	-	0.02%	0.01%	<0.01%
GLN	g+	g-	Og+		0.04%	0.02%	-	<0.01%	0.06%	0.13%	0.03%
GLN	g+	g-	Ng-		0.03%	0.01%	0.01%	<0.01%	0.07%	0.07%	0.03%
GLN	g+	g-	Ot		<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
GLN	t	g+	Ng+		0.45%	0.52%	0.36%	0.23%	0.55%	0.30%	0.38%
GLN	t	g+	Og-		0.20%	0.19%	0.13%	0.09%	0.33%	0.31%	0.15%
GLN	t	g+	Nt		0.12%	0.15%	0.10%	0.05%	0.11%	0.07%	0.09%
GLN	t	g+	Og+		0.65%	0.86%	0.45%	0.26%	0.61%	0.26%	0.27%
GLN	t	g+	Ng-		0.04%	0.05%	0.03%	0.01%	0.02%	0.02%	0.02%
GLN	t	g+	Ot		0.01%	0.01%	0.01%	<0.01%	0.01%	0.01%	<0.01%
GLN	t	t	Ng+		1.45%	1.38%	1.19%	1.20%	2.32%	1.28%	1.94%
GLN	t	t	Og-		1.74%	1.66%	1.70%	1.42%	2.67%	1.59%	2.21%
GLN	t	t	Nt		1.10%	1.10%	1.07%	0.62%	1.53%	1.11%	1.30%
GLN	t	t	Og+		2.09%	2.05%	1.93%	1.11%	3.31%	1.68%	2.85%
GLN	t	t	Ng-		1.43%	1.49%	1.41%	1.02%	1.91%	0.95%	1.88%
GLN	t	t	Ot		0.26%	0.25%	0.22%	0.22%	0.45%	0.19%	0.37%
GLN	t	g-	Ng+		0.01%	0.01%	0.01%	<0.01%	0.01%	<0.01%	0.01%
GLN	t	g-	Og-		0.14%	0.17%	0.13%	0.06%	0.16%	0.07%	0.21%
GLN	t	g-	Nt		0.04%	0.04%	0.06%	0.02%	0.04%	0.03%	0.04%
GLN	t	g-	Og+		0.06%	0.04%	0.03%	0.04%	0.13%	0.08%	0.05%
GLN	t	g-	Ng-		0.10%	0.11%	0.09%	0.07%	0.17%	0.07%	0.10%
GLN	t	g-	Ot		<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
GLN	g-	g+	Ng+		0.43%	0.48%	0.48%	0.47%	0.28%	0.40%	0.22%
GLN	g-	g+	Og-		0.83%	1.04%	0.32%	0.27%	0.42%	1.08%	0.16%
GLN	g-	g+	Nt		0.34%	0.39%	0.19%	0.09%	0.21%	0.56%	0.15%
GLN	g-	g+	Og+		0.45%	0.39%	0.48%	0.63%	0.57%	0.52%	0.50%
GLN	g-	g+	Ng-		0.01%	0.01%	0.01%	0.01%	0.02%	0.01%	0.01%
GLN	g-	g+	Ot		<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
GLN	g-	t	Ng+		10.84%	10.87%	11.33%	11.81%	10.14%	11.29%	9.94%
GLN	g-	t	Og-		17.59%	16.77%	18.73%	18.75%	17.49%	19.16%	18.26%
GLN	g-	t	Nt		10.62%	10.96%	10.28%	11.12%	9.10%	10.43%	9.79%
GLN	g-	t	Og+		20.10%	22.67%	17.62%	21.51%	15.16%	15.54%	18.49%
GLN	g-	t	Ng-		15.39%	14.85%	15.29%	20.08%	15.06%	15.71%	16.29%
GLN	g-	t	Ot		2.22%	2.15%	2.05%	2.65%	2.30%	2.45%	2.11%
GLN	g-	g-	Ng+		0.20%	0.15%	0.40%	0.21%	0.23%	0.21%	0.26%
GLN	g-	g-	Og-		3.83%	3.53%	6.54%	2.07%	3.89%	4.14%	4.13%
GLN	g-	g-	Nt		0.93%	0.91%	1.23%	0.41%	1.01%	1.05%	0.84%
GLN	g-	g-	Og+		1.26%	1.44%	1.04%	1.25%	0.77%	1.23%	0.53%
GLN	g-	g-	Ng-		2.54%	2.86%	2.57%	2.11%	1.50%	2.74%	1.19%
GLN	g-	g-	Ot		0.04%	0.04%	0.06%	0.02%	0.02%	0.02%	0.02%
GLU	g+	g+	g+		0.09%	0.06%	0.10%	<0.01%	0.08%	0.17%	0.02%
GLU	g+	g+	t		0.01%	0.01%	<0.01%	<0.01%	<0.01%	0.01%	<0.01%
GLU	g+	g+	g-		0.03%	0.01%	0.11%	<0.01%	0.07%	0.04%	<0.01%
GLU	g+	t	g+		1.31%	0.35%	1.41%	0.12%	3.22%	2.54%	4.01%
GLU	g+	t	t		0.32%	0.06%	0.34%	0.02%	1.02%	0.65%	0.70%
GLU	g+	t	g-		1.12%	0.30%	1.12%	0.15%	2.70%	2.51%	2.80%
GLU	g+	g-	g+		0.19%	0.12%	0.12%	<0.01%	0.13%	0.58%	0.04%
GLU	g+	g-	t		0.03%	0.02%	0.01%	<0.01%	0.02%	0.08%	<0.01%
GLU	g+	g-	g-		0.16%	0.06%	0.28%	0.01%	0.16%	0.45%	0.11%
GLU	t	g+	g+		1.69%	2.31%	1.00%	0.09%	1.06%	1.16%	0.44%
GLU	t	g+	t		0.34%	0.53%	0.19%	0.01%	0.12%	0.05%	0.04%
GLU	t	g+	g-		0.35%	0.37%	0.19%	0.13%	0.43%	0.43%	0.14%
GLU	t	t	g+		5.47%	6.50%	4.44%	2.64%	6.03%	2.92%	5.47%
GLU	t	t	t		1.59%	1.85%	1.22%	0.62%	1.92%	0.96%	1.49%
GLU	t	t	g-		6.06%	7.65%	4.73%	3.02%	5.65%	2.83%	4.55%
GLU	t	g-	g+		0.08%	0.08%	0.02%	0.07%	0.13%	0.10%	0.04%
GLU	t	g-	t		0.05%	0.05%	0.04%	<0.01%	0.08%	0.04%	<0.01%
GLU	t	g-	g-		0.71%	0.98%	0.30%	0.32%	0.48%	0.34%	0.17%
GLU	g-	g+	g+		1.22%	1.06%	1.05%	1.82%	0.85%	1.96%	0.90%
GLU	g-	g+	t		0.48%	0.51%	0.45%	0.03%	0.28%	0.71%	0.19%
GLU	g-	g+	g-		1.12%	1.12%	0.61%	0.66%	0.61%	1.96%	0.30%
GLU	g-	t	g+		25.45%	22.78%	30.66%	35.60%	26.51%	28.18%	29.13%
GLU	g-	t	t		12.73%	14.07%	10.60%	12.16%	11.47%	10.04%	11.02%
GLU	g-	t	g-		29.69%	26.24%	35.19%	39.41%	31.70%	33.47%	34.64%
GLU	g-	g-	g+		1.48%	1.96%	0.86%	0.76%	0.78%	1.23%	0.78%
GLU	g-	g-	t		1.28%	1.45%	0.95%	0.20%	1.27%	1.43%	0.80%
GLU	g-	g-	g-		6.97%	9.51%	4.03%	2.18%	3.22%	5.16%	2.18%
HID	g+	Ng+			2.31%	0.57%	2.20%	0.12%	4.74%	3.30%	1.79%
HID	g+	Cg-			1.46%	0.34%	1.82%	0.04%	3.52%	1.85%	0.37%
HID	g+	Nt			0.04%	<0.01%	<0.01%	<0.01%	0.03%	0.18%	0.01%
HID	g+	Cg+			2.59%	0.80%	3.08%	0.43%	5.61%	3.43%	0.74%
HID	g+	Ng-			1.78%	0.49%	2.96%	0.32%	3.87%	2.23%	0.75%
HID	g+	Ct			0.17%	<0.01%	<0.01%	0.01%	0.23%	0.72%	0.02%
HID	t	Ng+			14.91%	20.48%	11.88%	11.56%	12.07%	12.35%	11.66%
HID	t	Cg-			3.48%	4.79%	3.13%	2.48%	3.22%	2.28%	3.62%
HID	t	Nt			0.90%	1.11%	0.61%	0.85%	0.89%	0.45%	1.70%
HID	t	Cg+			9.56%	12.60%	9.20%	6.60%	7.83%	9.32%	4.80%
HID	t	Ng-			3.50%	4.00%	3.93%	4.53%	3.63%	2.53%	3.50%
HID	t	Ct			2.88%	3.66%	2.83%	2.84%	2.86%	1.17%	4.25%
HID	g-	Ng+			7.93%	8.75%	8.04%	5.62%	7.84%	7.03%	9.46%
HID	g-	Cg-			16.32%	14.86%	19.19%	21.20%	12.69%	16.47%	18.85%
HID	g-	Nt			2.00%	2.99%	1.19%	1.15%	1.10%	1.90%	0.74%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
HID	g-	Cg+			4.51%	3.31%	4.24%	5.00%	5.95%	5.87%	5.71%
HID	g-	Ng-			20.04%	14.89%	19.85%	31.65%	19.26%	23.93%	26.37%
HID	g-	Ct			5.62%	6.35%	5.84%	5.59%	4.66%	4.98%	5.67%
HIE	g+	Ng+			2.62%	1.76%	6.11%	0.01%	3.85%	1.79%	2.01%
HIE	g+	Cg-			0.81%	0.21%	2.19%	0.02%	2.35%	0.38%	0.51%
HIE	g+	Nt			0.01%	<0.01%	-	<0.01%	0.04%	0.01%	0.04%
HIE	g+	Cg+			2.58%	1.10%	2.38%	0.02%	4.19%	5.21%	3.65%
HIE	g+	Ng-			4.68%	5.15%	6.54%	0.01%	3.50%	4.85%	4.32%
HIE	g+	Ct			0.31%	0.25%	0.35%	-	0.35%	0.16%	0.13%
HIE	t	Ng+			13.17%	16.08%	8.79%	11.18%	13.62%	9.54%	11.11%
HIE	t	Cg-			3.04%	4.39%	2.18%	1.65%	2.71%	1.48%	2.20%
HIE	t	Nt			0.78%	1.06%	0.94%	0.44%	0.75%	0.11%	1.67%
HIE	t	Cg+			12.90%	15.17%	12.68%	4.10%	10.70%	15.45%	5.34%
HIE	t	Ng-			6.73%	5.73%	4.09%	3.69%	9.45%	10.19%	5.57%
HIE	t	Ct			4.20%	2.85%	2.40%	5.88%	7.09%	4.52%	1<0.01%
HIE	g-	Ng+			5.66%	6.31%	5.33%	5.58%	3.97%	6.41%	2.00%
HIE	g-	Cg-			16.20%	14.33%	24.23%	21.30%	13.42%	17.77%	18.41%
HIE	g-	Nt			1.98%	2.82%	2.19%	1.35%	1.01%	1.26%	1.20%
HIE	g-	Cg+			4.02%	2.94%	4.66%	6.66%	5.92%	3.21%	8.56%
HIE	g-	Ng-			16.03%	13.90%	13.16%	34.39%	15.18%	13.64%	22.04%
HIE	g-	Ct			4.29%	5.96%	1.77%	3.72%	1.90%	4.01%	1.26%
ILE	g+	g+			0.75%	0.55%	0.71%	0.01%	0.55%	1.51%	0.08%
ILE	g+	t			43.32%	22.67%	64.45%	14.42%	44.48%	71.16%	51.90%
ILE	g+	g-			0.10%	0.02%	0.10%	0.02%	0.14%	0.22%	0.11%
ILE	t	g+			0.98%	0.88%	1.56%	0.84%	1.25%	0.84%	1.09%
ILE	t	t			2.77%	1.20%	2.99%	0.19%	5.54%	2.81%	3.59%
ILE	t	g-			0.05%	0.05%	0.07%	0.01%	0.07%	0.04%	0.03%
ILE	g-	g+			0.36%	0.15%	0.29%	1.09%	0.78%	0.28%	0.84%
ILE	g-	t			28.55%	39.47%	10.93%	50.03%	3<0.01%	11.80%	29.70%
ILE	g-	g-			23.12%	35.01%	18.90%	33.39%	17.20%	11.34%	12.67%
LEU	g+	g+			0.26%	0.02%	0.19%	0.01%	0.87%	0.45%	0.06%
LEU	g+	t			0.19%	0.01%	0.17%	<0.01%	0.69%	0.23%	0.22%
LEU	g+	g-			<0.01%	<0.01%	<0.01%	<0.01%	0.01%	0.01%	<0.01%
LEU	t	g+			22.92%	24.48%	21.31%	15.88%	29.35%	14.13%	25.99%
LEU	t	t			3.26%	3.12%	3.25%	3.10%	5.29%	1.96%	4.36%
LEU	t	g-			1.19%	1.49%	1.64%	0.58%	1.12%	0.44%	0.82%
LEU	g-	g+			4.18%	2.71%	4.14%	4.50%	7.46%	5.70%	6.65%
LEU	g-	t			66.49%	66.45%	67.31%	75.00%	54.11%	75.59%	61.27%
LEU	g-	g-			1.51%	1.71%	1.99%	0.92%	1.11%	1.49%	0.63%
LYS	g+	g+	g+	g+	0.01%	<0.01%	<0.01%	-	0.03%	0.01%	<0.01%
LYS	g+	g+	g+	t	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g+	g+	g+	g-	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g+	g+	t	g+	0.06%	0.03%	0.13%	<0.01%	0.06%	0.14%	0.01%
LYS	g+	g+	t	t	0.01%	0.01%	0.01%	-	0.01%	0.04%	<0.01%
LYS	g+	g+	t	g-	0.08%	0.06%	0.06%	<0.01%	0.10%	0.13%	<0.01%
LYS	g+	g+	g-	g+	<0.01%	-	-	-	<0.01%	<0.01%	-
LYS	g+	g+	g-	t	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	-
LYS	g+	g+	g-	g-	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g+	t	g+	g+	0.22%	0.03%	0.22%	0.01%	0.62%	0.39%	0.24%
LYS	g+	t	g+	t	0.14%	0.02%	0.05%	<0.01%	0.42%	0.31%	0.18%
LYS	g+	t	g+	g-	0.01%	<0.01%	<0.01%	<0.01%	0.01%	<0.01%	<0.01%
LYS	g+	t	t	g+	2.25%	1.03%	2.63%	0.18%	3.47%	4.10%	3.01%
LYS	g+	t	t	t	0.43%	0.07%	0.12%	<0.01%	1.50%	0.91%	0.27%
LYS	g+	t	t	g-	1.21%	0.38%	1.80%	0.11%	2.68%	2.13%	1.32%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
LYS	g+	t	g-	g+	0.01%	<0.01%	0.03%	<0.01%	0.01%	0.01%	0.01%
LYS	g+	t	g-	t	0.13%	0.02%	0.05%	<0.01%	0.34%	0.33%	0.14%
LYS	g+	t	g-	g-	0.52%	0.15%	0.63%	0.02%	1.05%	1.16%	0.56%
LYS	g+	g-	g+	g+	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g+	g-	g+	t	<0.01%	-	<0.01%	-	<0.01%	<0.01%	-
LYS	g+	g-	g+	g-	-	-	-	-	-	-	-
LYS	g+	g-	t	g+	0.02%	<0.01%	0.01%	<0.01%	0.09%	0.02%	0.05%
LYS	g+	g-	t	t	<0.01%	<0.01%	<0.01%	<0.01%	0.01%	<0.01%	<0.01%
LYS	g+	g-	t	g-	0.02%	0.01%	0.08%	<0.01%	0.04%	0.02%	0.02%
LYS	g+	g-	g-	g+	<0.01%	-	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g+	g-	g-	t	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	g+	g-	g-	g-	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g+	g+	g+	0.22%	0.29%	0.27%	0.09%	0.14%	0.18%	0.09%
LYS	t	g+	g+	t	0.19%	0.31%	0.07%	0.07%	0.10%	0.04%	0.11%
LYS	t	g+	g+	g-	<0.01%	0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g+	t	g+	2.02%	2.54%	1.93%	1.15%	1.84%	0.90%	2.72%
LYS	t	g+	t	t	0.29%	0.42%	0.17%	0.09%	0.22%	0.12%	0.29%
LYS	t	g+	t	g-	1.42%	1.78%	1.12%	0.64%	1.37%	0.89%	1.26%
LYS	t	g+	g-	g+	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g+	g-	t	0.03%	0.06%	0.01%	0.01%	0.01%	<0.01%	0.01%
LYS	t	g+	g-	g-	0.04%	0.06%	0.02%	0.05%	0.02%	0.01%	0.07%
LYS	t	t	g+	g+	2.32%	3.04%	1.67%	1.05%	2.11%	1.21%	1.85%
LYS	t	t	g+	t	0.87%	1.17%	0.26%	0.12%	1.01%	0.47%	1.07%
LYS	t	t	g+	g-	0.03%	0.03%	0.02%	0.02%	0.02%	0.02%	0.01%
LYS	t	t	t	g+	3.52%	3.72%	3.12%	1.69%	4.85%	2.31%	6.09%
LYS	t	t	t	t	0.77%	0.75%	0.37%	0.28%	1.39%	0.73%	0.87%
LYS	t	t	t	g-	4.81%	5.95%	3.14%	3.82%	4.90%	2.55%	5.87%
LYS	t	t	g-	g+	0.02%	<0.01%	<0.01%	0.01%	0.06%	0.04%	0.01%
LYS	t	t	g-	t	0.36%	0.39%	0.27%	0.13%	0.47%	0.36%	0.27%
LYS	t	t	g-	g-	0.53%	0.54%	0.54%	0.31%	0.79%	0.35%	0.81%
LYS	t	g-	g+	g+	0.01%	0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g-	g+	t	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g-	g+	g-	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	-	<0.01%
LYS	t	g-	t	g+	0.30%	0.40%	0.21%	0.16%	0.32%	0.12%	0.38%
LYS	t	g-	t	t	0.07%	0.08%	0.05%	0.04%	0.07%	0.03%	0.06%
LYS	t	g-	t	g-	0.52%	0.70%	0.40%	0.23%	0.48%	0.13%	0.78%
LYS	t	g-	g-	g+	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	t	g-	g-	t	0.06%	0.08%	0.05%	<0.01%	0.05%	0.02%	0.04%
LYS	t	g-	g-	g-	0.15%	0.20%	0.08%	0.05%	0.18%	0.05%	0.15%
LYS	g-	g+	g+	g+	0.11%	0.07%	0.11%	0.29%	0.12%	0.16%	0.08%
LYS	g-	g+	g+	t	0.03%	0.04%	0.04%	0.05%	0.03%	0.02%	0.03%
LYS	g-	g+	g+	g-	<0.01%	<0.01%	<0.01%	0.02%	0.01%	0.01%	0.01%
LYS	g-	g+	t	g+	0.61%	0.58%	1.07%	0.46%	0.66%	0.54%	0.59%
LYS	g-	g+	t	t	0.06%	0.05%	0.06%	0.07%	0.06%	0.05%	0.06%
LYS	g-	g+	t	g-	0.39%	0.37%	0.48%	0.36%	0.44%	0.43%	0.45%
LYS	g-	g+	g-	g+	<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
LYS	g-	g+	g-	t	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%	<0.01%
LYS	g-	g+	g-	g-	0.01%	0.02%	0.01%	<0.01%	<0.01%	0.01%	<0.01%
LYS	g-	t	g+	g+	4.79%	4.56%	4.27%	4.89%	4.94%	5.49%	5.01%
LYS	g-	t	g+	t	2.01%	2.35%	0.91%	1.42%	1.83%	2.15%	1.44%
LYS	g-	t	g+	g-	0.09%	0.08%	0.04%	0.12%	0.08%	0.10%	0.21%
LYS	g-	t	t	g+	14.99%	13.34%	16.48%	24.88%	14.52%	16.08%	15.10%
LYS	g-	t	t	t	4.96%	6.42%	2.50%	3.23%	3.49%	4.39%	2.88%
LYS	g-	t	t	g-	22.34%	23.16%	22.72%	25.24%	19.66%	21.00%	21.22%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
LYS	g-	t	g-	g+	0.19%	0.21%	0.20%	0.23%	0.09%	0.23%	0.09%
LYS	g-	t	g-	t	3.67%	4.51%	1.58%	2.64%	2.90%	3.72%	2.39%
LYS	g-	t	g-	g-	5.13%	3.62%	5.88%	12.35%	5.32%	6.37%	5.76%
LYS	g-	g-	g+	g+	0.26%	0.41%	0.18%	0.03%	0.09%	0.11%	0.07%
LYS	g-	g-	g+	t	0.09%	0.15%	0.05%	0.02%	0.03%	0.04%	0.02%
LYS	g-	g-	g+	g-	<0.01%	<0.01%	<0.01%	0.03%	<0.01%	<0.01%	<0.01%
LYS	g-	g-	t	g+	6.06%	6.26%	6.70%	4.86%	4.97%	6.88%	4.88%
LYS	g-	g-	t	t	1.04%	1.03%	1.24%	0.73%	0.96%	1.24%	0.68%
LYS	g-	g-	t	g-	7.64%	6.31%	13.94%	6.52%	7.44%	8.85%	9.19%
LYS	g-	g-	g-	g+	0.02%	0.02%	0.01%	0.01%	0.01%	0.02%	0.01%
LYS	g-	g-	g-	t	0.66%	0.82%	0.56%	0.21%	0.54%	0.65%	0.33%
LYS	g-	g-	g-	g-	1.19%	1.25%	1.30%	1.02%	0.99%	1.20%	0.85%
MET	g+	g+	g+		0.07%	0.01%	0.08%	<0.01%	0.20%	0.15%	<0.01%
MET	g+	g+	t		0.07%	0.01%	0.06%	<0.01%	0.22%	0.12%	0.01%
MET	g+	g+	g-		<0.01%	<0.01%	<0.01%	-	<0.01%	<0.01%	<0.01%
MET	g+	t	g+		0.73%	0.06%	0.58%	0.06%	2.28%	1.37%	0.79%
MET	g+	t	t		0.76%	0.06%	0.72%	0.07%	2.40%	1.41%	0.53%
MET	g+	t	g-		0.79%	0.08%	1.09%	0.04%	2.13%	1.93%	0.47%
MET	g+	g-	g+		<0.01%	<0.01%	<0.01%	-	<0.01%	0.01%	-
MET	g+	g-	t		0.08%	<0.01%	0.04%	<0.01%	0.25%	0.23%	0.02%
MET	g+	g-	g-		0.07%	<0.01%	0.03%	<0.01%	0.32%	0.09%	0.02%
MET	t	g+	g+		1.92%	2.44%	2.27%	0.98%	1.55%	1.11%	1.30%
MET	t	g+	t		2.17%	2.94%	2.33%	0.74%	1.60%	0.93%	1.33%
MET	t	g+	g-		0.09%	0.12%	0.07%	0.05%	0.06%	0.02%	0.09%
MET	t	t	g+		4.50%	5.14%	3.35%	2.06%	5.26%	3.07%	5.00%
MET	t	t	t		2.53%	2.39%	2.98%	1.56%	3.71%	1.90%	3.90%
MET	t	t	g-		2.55%	2.45%	2.55%	1.91%	3.79%	1.86%	3.67%
MET	t	g-	g+		0.01%	0.01%	0.01%	0.01%	0.01%	<0.01%	0.02%
MET	t	g-	t		0.52%	0.72%	0.65%	0.21%	0.31%	0.16%	0.46%
MET	t	g-	g-		1.16%	1.80%	0.99%	0.15%	0.54%	0.29%	0.62%
MET	g-	g+	g+		0.72%	0.33%	1.14%	1.47%	1.04%	1.27%	1.25%
MET	g-	g+	t		0.83%	0.65%	1.11%	1.09%	0.94%	1.08%	1.30%
MET	g-	g+	g-		0.03%	0.04%	0.02%	0.01%	0.01%	0.03%	0.01%
MET	g-	t	g+		16.40%	15.74%	14.54%	18.44%	17.15%	17.31%	18.70%
MET	g-	t	t		15.82%	14.04%	13.67%	18.81%	17.96%	18.65%	19.40%
MET	g-	t	g-		20.74%	18.91%	18.42%	31.16%	22.10%	22.81%	24.69%
MET	g-	g-	g+		0.94%	1.36%	0.57%	0.30%	0.29%	0.65%	0.16%
MET	g-	g-	t		11.48%	12.98%	13.23%	9.51%	7.09%	10.57%	7.49%
MET	g-	g-	g-		15.06%	17.72%	19.49%	11.37%	8.77%	13.00%	8.76%
PHE	g+	g			6.47%	0.82%	7.04%	0.23%	15.79%	9.44%	3.27%
PHE	g+	t			0.02%	<0.01%	0.04%	<0.01%	0.03%	0.03%	0.01%
PHE	t	g			39.54%	59.47%	39.89%	22.88%	25.89%	20.18%	30.21%
PHE	t	t			2.79%	3.67%	2.14%	3.15%	2.40%	0.89%	5.15%
PHE	g-	g			45.99%	29.79%	47.36%	69.48%	52.54%	63.16%	58.75%
PHE	g-	t			5.19%	6.25%	3.53%	4.26%	3.35%	6.30%	2.61%
PRO	g+				62.93%	58.04%	97.66%	-	81.32%	65.62%	100.00%
PRO	g-				37.07%	41.96%	2.34%	100.00%	18.68%	34.38%	-
SER	g+				22.69%	14.33%	19.70%	1.91%	31.69%	34.91%	26.59%
SER	t				2.05%	1.30%	1.98%	2.39%	3.91%	1.95%	4.36%
SER	g-				75.25%	84.37%	78.31%	95.70%	64.40%	63.14%	69.04%
THR	g+				45.14%	26.50%	55.71%	13.97%	52.54%	61.66%	57.70%
THR	t				1.71%	0.12%	0.93%	0.36%	4.84%	1.46%	4.78%
THR	g-				53.15%	73.38%	43.36%	85.67%	42.63%	36.88%	37.52%
TRP	g+	g+			6.57%	4.05%	14.85%	0.05%	11.08%	5.98%	1.85%

Residue	χ1	χ2	χ3	χ4	BBIND	RSS α_R	RSS Near α_R	RSS α_L	RSS β	RSS P_{IIL}	RSS P_{IR}
TRP	g+	t			0.51%	0.06%	0.16%	<0.01%	0.86%	1.38%	0.37%
TRP	g+	g-			3.94%	0.95%	5.75%	0.05%	8.22%	5.83%	3.66%
TRP	t	g+			16.59%	22.66%	15.48%	10.69%	10.90%	12.05%	11.85%
TRP	t	t			10.53%	12.39%	8.80%	7.45%	11.17%	4.74%	22.51%
TRP	t	g-			13.28%	21.20%	10.92%	2.88%	8.47%	5.17%	6.12%
TRP	g-	g+			7.19%	3.20%	8.98%	22.40%	9.20%	9.08%	16.93%
TRP	g-	t			14.98%	14.92%	12.51%	17.46%	11.15%	20.57%	11.69%
TRP	g-	g-			26.40%	20.56%	22.55%	39.01%	28.94%	35.20%	25.03%
TYR	g+	g			8.27%	1.44%	8.56%	0.70%	18.84%	11.34%	4.28%
TYR	g+	t			0.02%	<0.01%	<0.01%	<0.01%	0.04%	0.04%	0.08%
TYR	t	g			37.99%	57.87%	35.08%	26.01%	24.75%	21.51%	25.61%
TYR	t	t			2.85%	3.88%	1.67%	2.40%	2.38%	0.98%	5.63%
TYR	g-	g			45.57%	30.22%	51.02%	68.31%	50.71%	59.62%	61.07%
TYR	g-	t			5.29%	6.60%	3.66%	2.58%	3.29%	6.52%	3.33%
VAL	g+				1.36%	0.71%	1.19%	0.18%	2.32%	1.41%	1.33%
VAL	t				55.53%	81.10%	43.65%	89.09%	50.17%	26.78%	48.76%
VAL	g-				43.11%	18.19%	55.16%	10.73%	47.51%	71.81%	49.91%

Table S2: (Related to Figure 7) Rotamer definitions for rotameric and non-rotameric χ-angles.

Residue	# χ angles	Rotamer Structure	# Rotameric rotamers	Non-rotameric angles	# Non-rotameric χ bins	Total # rotamers
ARG	4	χ1,χ2,χ3,χ4	81	-	-	81
ASN	2	χ1,χ2	3	χ2	6	18
ASP	2	χ1,χ2	3	χ2	6	18
CYS	2	χ1	3		-	3
GLN	3	χ1,χ2,χ3	9	χ3	6	54
GLU	3	χ1,χ2,χ3	9	χ3	6	54
HIS	2	χ1,χ2	3	χ2	6	18
ILE	2	χ1,χ2	9	-	-	9
LEU	2	χ1,χ2	9	-	-	9
LYS	3	χ1,χ2,χ3,χ4	81	-	-	81
MET	4	χ1,χ2,χ3	27	-	-	27
PHE	2	χ1,χ2	3	χ2	4	12
PRO	1	χ1	-	χ1	2	2
SER	1	χ1	3	-	-	3
THR	1	χ1	3	-	-	3
TRP	2	χ1,χ2	9	-	-	9
TYR	2	χ1,χ2	3	χ2	4	12
VAL	1	χ1	3	-	-	3