SUPPLEMENTARY INFORMATION:

Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins

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Table 1: Parameters for hydrophobic side-chain models interacting with ions.

Ca^{2+}								
	ala	pro	val	leu	ile	phe	met	trp
ε_{ij}^{0} [kcal/mol]	1.68E-01	1.67E+00	1.13E+00	1.97E-01	2.21E+00	3.47E-02	3.47E-02	4.43E-02
σ_{ij}^{0} [Å]	4.16E+00	2.45E+00	3.88E+00	5.10E+00	4.07E+00	5.73E+00	5.70E+00	5.96E+00
χ_{ij}	5.69E-01	5.27E-01	4.97E-01	2.69E-01	4.78E-01	4.22E-01	4.05E-01	6.22E-01
χ'_{ij}	9.48E-01	-9.99E-01	4.08E-01	-4.53E-01	5.41E-01	7.66E-01	-9.99E-01	6.60E-01
σ [Å]	2.57E+00	2.78E+00	2.95E+00	2.70E+00	3.60E+00	3.23E+00	8.11E+00	3.01E+00
$\chi_{ij}^{\prime\prime(1)}$	-8.29E-02	3.36E-01	8.60E-02	6.80E-01	8.78E-03	6.50E-01	5.25E-01	4.88E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	8.97E+00	3.75E+00	5.56E+00	4.00E+00	2.39E+00	1.97E+00	1.17E-01	5.00E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	5.80E+00	2.65E+00	4.56E+00	3.00E+00	1.88E+00	1.28E+00	5.94E+00	5.00E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	6.95E+00	3.47E-02	2.80E+00	4.65E-02	8.20E-02	3.47E-02	3.70E+00	5.00E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	3.47E-02	3.47E-02	3.47E-02	5.05E-01	5.91E-02	7.89E-01	4.62E+00	5.00E+00
Mg^{2+}								
	ala	pro	val	leu	ile	phe	met	trp
ε_{ij}^{0} [kcal/mol]	2.07E-01	5.17E-01	3.47E-02	3.47E-02	3.47E-02	3.48E-02	5.12E+00	3.47E-02
σ_{ij}^{0} [Å]	4.26E+00	4.03E+00	5.54E+00	5.80E+00	5.80E+00	5.14E+00	2.97E+00	6.44E+00
χ_{ij}	3.77E-01	6.11E-02	9.57E-02	3.90E-01	3.28E-01	9.02E-02	7.88E-01	5.93E-01
χ'_{ij}	5.43E-01	-9.99E-01	-8.07E-01	2.94E-02	3.23E-01	-7.76E-02	2.06E-01	7.38E-01

σ [Å]	2.56E+00	3.23E+00	4.92E+00	4.12E+00	4.52E+00	4.64E+00	4.32E+00	3.07E+00
$\chi_{ij}^{\prime\prime(1)}$	6.34E-02	3.49E-01	5.32E-01	1.87E-01	-3.32E-02	5.23E-01	5.87E-01	4.90E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	8.38E+00	3.53E+00	1.03E-01	1.55E+00	7.86E-01	5.97E-01	3.01E+00	5.00E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	5.13E+00	2.85E+00	1.93E-01	9.03E-01	4.19E+00	6.73E+00	7.15E+00	5.00E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	6.83E+00	4.14E-02	2.99E-01	3.67E-02	1.94E+00	3.16E+00	8.29E-01	5.00E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	3.48E-02	1.75E-01	2.62E-01	2.24E-01	4.02E-01	4.89E+00	4.85E+00	5.00E+00

K^+								
	ala	pro	val	leu	ile	phe	met	trp
ε_{ij}^0 [kcal/mol]	4.33E-02	3.51E-02	5.68E-01	3.50E-02	3.59E-02	2.62E+00	5.62E-02	4.51E-02
σ_{ij}^0 [Å]	4.32E+00	4.16E+00	3.87E+00	5.19E+00	4.72E+00	2.90E+00	4.43E+00	4.56E+00
χ_{ij}	4.68E-01	2.59E-01	3.04E-01	2.65E-01	2.02E-01	7.19E-01	5.27E-01	5.86E-01
χ'_{ij}	9.27E-01	-7.36E-01	-5.45E-01	1.09E-01	-2.35E-01	9.99E-01	-9.36E-01	6.42E-01
σ [Å]	3.11E+00	3.74E+00	4.49E+00	4.16E+00	4.03E+00	4.93E+00	4.39E+00	4.78E+00
$\chi_{ij}^{\prime\prime(1)}$	2.43E-01	2.35E-01	3.43E-01	3.36E-01	8.92E-02	2.83E-01	6.44E-01	4.18E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	6.99E+00	1.15E+00	1.19E+00	6.58E-01	7.11E-01	6.22E-01	3.94E+00	2.98E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	4.18E+00	5.46E-01	6.77E-01	3.00E-01	4.36E-01	6.71E+00	5.63E+00	5.32E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	5.94E+00	2.59E-01	3.47E-02	6.08E-02	6.13E-02	7.60E-01	5.69E+00	5.46E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	4.44E-01	4.43E-01	3.73E-01	2.58E-01	7.85E-02	4.71E+00	5.02E+00	4.93E+00
Na^+								
	ala	pro	val	leu	ile	phe	met	trp
ε_{ij}^0 [kcal/mol]	2.79E-01	3.48E-02	3.50E-02	3.52E-02	3.49E-02	1.46E+00	2.79E+00	3.47E-02
σ_{ij}^0 [Å]	3.38E+00	4.01E+00	4.35E+00	4.64E+00	4.37E+00	2.84E+00	2.92E+00	2.97E+00
χ_{ij}	4.59E-01	1.98E-01	2.09E-01	3.64E-01	2.59E-01	7.43E-01	8.34E-01	4.04E-01
χ'_{ij}	9.10E-01	-8.63E-01	6.64E-03	1.59E-01	-9.68E-02	1.00E+00	1.00E+00	-1.00E+00
σ [Å]	2.51E+00	3.70E+00	4.12E+00	4.11E+00	3.82E+00	4.56E+00	4.44E+00	4.09E+00

$\chi_{ij}^{\prime\prime(1)}$	1.49E-01	2.87E-01	1.62E-01	4.01E-01	2.49E-01	3.76E-01	4.32E-01	6.96E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	8.34E+00	1.49E+00	1.37E+00	9.54E-01	1.35E+00	5.99E-01	9.82E-01	5.19E-01
$\alpha_{ij}^{(2)}$ [kcal/mol]	4.99E+00	9.07E-01	7.15E-01	4.77E-01	8.43E-01	6.56E+00	6.93E+00	1.20E+01
$\alpha_{ij}^{(3)}$ [kcal/mol]	6.91E+00	2.76E-01	3.47E-02	3.47E-02	3.47E-02	3.47E-02	5.97E-01	3.47E-02
$\alpha_{ij}^{(4)}$ [kcal/mol]	8.14E-02	3.93E-01	6.56E-01	2.68E-01	2.60E-01	4.74E+00	4.88E+00	4.46E+00

Cl^-								
	ala	pro	val	leu	ile	phe	met	trp
ε_{ij}^0 [kcal/mol]	3.47E-02	1.20E-01	3.75E-02	3.47E-02	3.47E-02	2.73E+00	3.47E-02	3.47E-02
σ_{ij}^0 [Å]	5.14E+00	4.37E+00	5.09E+00	5.10E+00	5.10E+00	2.59E+00	4.46E+00	2.78E+00
χ_{ij}	3.09E-01	2.52E-01	1.56E-01	4.71E-01	5.04E-01	1.00E+00	5.13E-01	1.00E+00
χ'_{ij}	7.55E-01	-1.00E+00	-7.28E-01	4.97E-01	8.92E-01	1.00E+00	-8.91E-01	-1.00E+00
σ [Å]	3.18E+00	4.45E+00	4.76E+00	4.24E+00	4.06E+00	3.02E+00	3.89E+00	4.25E+00
$\chi_{ij}^{\prime\prime(1)}$	7.72E-02	3.82E-01	2.44E-01	2.25E-02	-2.09E-02	2.44E-01	5.21E-01	5.55E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	8.65E+00	8.30E-01	5.36E-01	6.72E-01	6.60E-01	1.44E+01	6.42E+00	2.45E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	4.56E+00	3.60E-02	6.28E-02	3.31E-01	3.60E-01	5.14E+00	7.07E+00	6.02E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	7.60E+00	1.54E-01	3.47E-02	7.56E-02	3.49E-02	6.68E-01	6.10E+00	3.53E-02
$\alpha_{ij}^{(4)}$ [kcal/mol]	2.16E-01	1.23E-01	4.22E-02	8.67E-02	4.60E-02	1.14E+00	4.90E+00	5.51E+00

Table 2: Parameters for polar side-chain models and peptide-group interacting with ions.

Ca^{2+}								
	ser	thr	cys	asn	gln	his	tyr	pept
ε_{ij}^{0} [kcal/mol]	6.76E+00	5.09E+00	9.98E-01	3.87E+00	2.45E+00	1.35E+00	2.60E+00	8.59E+00
σ_{ij}^{0} [Å]	2.76E+00	3.15E+00	4.18E+00	2.92E+00	3.90E+00	3.12E+00	3.70E+00	2.91E+00
χ_{ij}	2.47E-01	7.42E-02	6.77E-01	8.36E-01	6.41E-01	5.92E-01	4.46E-01	4.75E-01
χ'_{ij}	-1.09E-01	1.81E-01	9.97E-01	1.00E+00	8.05E-01	1.00E+00	-4.18E-01	4.69E-01
σ [Å]	4.57E+00	4.85E+00	4.79E+00	4.77E+00	2.22E+00	4.60E+00	3.76E+00	4.67E+00
$\chi_{ij}^{\prime\prime(1)}$	2.36E-01	5.71E-02	9.56E-02	3.57E-01	-5.53E-02	-5.19E-01	5.42E-01	3.26E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	2.14E+00	4.81E+00	7.32E-01	3.60E+00	3.20E+00	1.24E+00	2.10E+01	5.27E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	4.84E+00	6.53E+00	5.99E+00	5.60E+00	6.31E+00	4.70E+00	1.58E+01	3.05E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	3.44E-01	4.53E+00	5.13E-01	4.48E+00	1.83E+00	1.44E+00	1.51E+01	2.01E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	5.02E+00	5.17E+00	5.16E+00	5.22E+00	5.31E+00	5.28E+00	3.44E+00	4.96E+00
d_{head} [Å]	3.78E-01	5.04E-02	4.66E-02	7.33E-02	3.58E-02	4.45E-02	3.47E-02	1.66E-01
a_i	9.99E-01	7.56E-02	3.57E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	1.00E+00
ϵ_{in}	1.37E+00	1.00E+01	1.16E+00	1.04E+00	1.18E+00	9.87E+00	9.34E-01	1.00E+00
α_{ij}^{pol}	7.49E-02	3.60E-01	1.77E+00	1.85E+00	1.87E+00	3.25E+00	7.80E-01	3.50E-02
$w_{\perp}$	-2.97E+00	-4.07E+00	-4.26E+00	-2.18E+00	-3.35E+00	-8.01E+00	-1.30E+01	-4.64E+00
$w_{\parallel}$	1.67E+00	4.09E-01	3.61E-02	3.95E-02	1.16E-01	1.81E+01	1.84E+00	3.47E-02

Mg^{2+}								
	ser	thr	cys	asn	gln	his	tyr	pept
ε_{ij}^{0} [kcal/mol]	3.50E-02	2.89E+00	5.40E-01	4.00E+00	2.02E+00	5.17E-01	6.03E+00	1.03E+01
σ_{ij}^{0} [Å]	3.43E+00	2.92E+00	4.42E+00	3.02E+00	3.10E+00	4.63E+00	2.59E+00	3.01E+00
χ_{ij}	2.70E-01	1.06E-01	6.41E-01	3.37E-01	3.35E-01	7.30E-01	8.10E-01	3.54E-01
$\chi_{ij}^{\prime}$	4.40E-01	1.91E-01	9.57E-01	2.61E-01	5.51E-01	1.00E+00	1.00E+00	3.33E-01
σ [Å]	4.33E+00	4.49E+00	3.26E+00	4.73E+00	4.75E+00	4.42E+00	4.09E+00	4.57E+00
$\chi_{ij}^{\prime\prime(1)}$	3.67E-01	7.36E-02	-5.41E-01	2.66E-01	2.74E-01	2.84E-01	6.49E-01	2.82E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	3.51E+00	4.94E+00	1.42E+00	4.02E+00	2.25E+00	2.43E+00	3.48E+00	8.07E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	6.12E+00	6.67E+00	5.84E+00	5.61E+00	5.05E+00	5.10E+00	6.84E+00	5.46E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	4.18E+00	4.70E+00	2.22E+00	4.16E+00	3.93E+00	1.37E+00	8.29E-02	4.09E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	5.24E+00	5.18E+00	5.28E+00	5.20E+00	5.30E+00	5.27E+00	5.19E+00	4.78E+00
d_{head} [Å]	3.47E-02	3.47E-02	5.60E-02	1.38E-01	8.01E-01	1.55E-01	3.47E-02	3.53E-02
a_i	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	1.00E+00
ϵ_{in}	1.00E+01	1.00E+01	9.88E+00	1.57E+00	1.35E+00	1.68E+00	2.79E+00	1.00E+00
α_{ij}^{pol}	9.44E-01	3.54E-01	2.98E+00	3.47E-02	5.36E-02	1.63E+00	1.70E-01	3.51E-02
$w_{\perp}$	-2.65E+00	-3.63E+00	-2.41E+00	-7.74E+00	-6.64E+00	-6.72E+00	-3.41E+00	-3.82E+00
$w_{\parallel}$	3.66E-02	1.27E-01	3.97E-02	1.89E+00	6.17E-01	1.80E+01	3.47E-02	3.47E-02
K^{+}								

	ser	thr	cys	asn	gln	his	tyr	pept
ε_{ij}^{0} [kcal/mol]	4.56E-02	3.07E+00	2.28E+00	4.56E+00	3.79E+00	3.57E+00	1.29E+00	6.09E+00
σ_{ij}^{0} [Å]	3.98E+00	3.15E+00	3.12E+00	3.21E+00	3.04E+00	2.91E+00	3.57E+00	3.11E+00
χ_{ij}	4.43E-01	6.82E-01	7.53E-01	7.64E-01	8.27E-01	8.57E-01	7.04E-01	7.44E-01
χ_{ij}'	8.59E-01	9.99E-01	9.96E-01	1.00E+00	9.95E-01	1.00E-00	1.76E-01	1.00E+00
σ [Å]	3.54E+00	4.89E+00	4.58E+00	5.02E+00	4.62E+00	4.73E+00	4.28E+00	5.10E+00
$\chi_{ij}^{\prime\prime(1)}$	1.96E-01	-2.36E-01	7.68E-02	-7.60E-02	2.17E-01	3.72E-01	5.38E-01	-2.42E-02
$\alpha_{ij}^{(1)}$ [kcal/mol]	1.10E+01	2.61E+00	2.18E+00	1.89E+00	2.04E+00	9.74E-01	8.02E+00	1.16E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	8.19E+00	5.54E+00	5.60E+00	5.77E+00	5.82E+00	4.70E+00	7.47E+00	5.51E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	8.80E+00	3.91E+00	3.52E+00	2.86E+00	2.85E+00	8.84E-02	7.07E+00	2.87E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	4.89E+00	5.21E+00	5.23E+00	5.18E+00	5.21E+00	5.26E+00	5.16E+00	5.27E+00
d_{head} [Å]	0.00E+00	2.01E-01	2.76E-01	3.47E-02	3.47E-02	9.68E-01	3.47E-02	3.80E-02
a_i	1.00E+01	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02
ϵ_{in}	9.84E-01	9.96E+00	9.95E+00	9.95E+00	9.89E+00	9.91E+00	1.00E+01	1.20E+00
α_{ij}^{pol}	4.01E-01	1.61E+00	1.88E+00	2.01E+00	2.87E+00	3.13E+00	3.47E-02	2.19E+00
$w_{\perp}$	-3.33E+00	-5.63E+00	-7.74E+00	-3.99E+00	-5.14E+00	-1.18E+01	-1.80E+01	-6.35E+00
$w_{\parallel}$	2.37E-01	1.03E-01	9.51E-02	9.96E-02	9.66E-02	1.83E+01	5.32E+01	3.87E-02
Na^{+}								
	ser	thr	cys	asn	gln	his	tyr	pept

ε_{ij}^{0} [kcal/mol]	2.33E-01	7.58E+00	5.70E-02	1.90E-01	9.48E+00	3.47E-02	4.23E-02	3.84E+00
σ_{ij}^{0} [Å]	2.97E+00	2.69E+00	3.17E+00	1.96E+00	2.90E+00	3.49E+00	3.55E+00	2.72E+00
χ_{ij}	4.54E-01	6.59E-01	4.95E-01	1.00E+00	7.84E-01	1.78E-01	7.52E-01	7.07-01
χ'_{ij}	7.25E-01	9.97E-01	8.10E-01	9.98E-01	9.99E-01	-4.61E-01	1.00E+00	1.00E+00
σ [Å]	3.79E+00	4.40E+00	4.43E+00	4.34E+00	4.42E+00	3.30E+00	4.15E+00	4.19E+00
$\chi_{ij}^{\prime\prime(1)}$	2.46E-01	4.44E-02	4.14E-01	4.02E-01	3.36E-01	4.50E-01	4.92E-01	4.89E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	8.23E+00	2.25E+00	5.96E-01	7.38E-01	3.43E+00	7.67E-01	1.46E+00	1.55E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	5.44E+00	5.92E+00	5.61E+00	6.05E+00	6.23E+00	5.49E-01	8.57E-01	5.23E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	4.89E+00	2.69E+00	2.58E+00	6.70E-01	3.00E+00	1.78E-01	1.46E-01	3.53E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	4.96E+00	5.21E+00	5.23E+00	5.20E+00	5.18E+00	3.47E-02	2.12E+00	5.30E+00
d_{head} [Å]	3.47E-02	4.02E-02	4.13E-02	4.72E-02	1.47E-01	5.53E-02	3.47E-02	3.53E-02
a_i	1.00E+00	7.56E-02	7.56E-02	7.56E-02	7.56E-02	3.47E-02	3.47E-02	7.37E-02
ϵ_{in}	1.00E+00	1.08E+00	1.35E+00	9.67E-01	9.47E-01	1.00E+00	1.00E+00	1.15E+00
α_{ij}^{pol}	4.59E-02	1.50E+00	9.69E-01	1.89E+00	1.91E+00	3.47E-02	3.47E-02	1.43E+00
$w_{\perp}$	-7.67E-01	-3.68E+00	-9.04E+00	-1.51E+00	3.95E+00	-1.04E+01	-3.18E-02	2.00E+00
$w_{\parallel}$	1.90E-01	1.80E-01	3.63E-02	1.59E-01	4.00E-01	6.06E-01	1.03E-01	4.10E-01
Cl^{-}								
	ser	thr	cys	asn	gln	his	tyr	pept
ε_{ij}^{0} [kcal/mol]	3.48E-02	4.82E+00	8.62E-01	1.61E+00	2.20E+00	3.42E+00	3.48E-02	3.47E-02

σ_{ij}^{0} [Å]	4.53E+00	3.41E+00	3.73E+00	3.72E+00	2.97E+00	1.23E+00	5.16E+00	4.60E+00
χ_{ij}	5.72E-01	6.65E-01	7.01E-01	7.24E-01	5.25E-01	9.14E-01	6.75E-01	6.70E-01
χ'_{ij}	1.00E+00	9.97E-01	9.89E-01	1.00E+00	9.94E-01	1.00E+00	1.00E+00	9.99E-01
σ [Å]	4.08E+00	5.29E+00	6.23E+00	6.48E+00	3.88E+00	3.56E+00	5.02E+00	1.31E+00
$\chi_{ij}^{\prime\prime(1)}$	4.69E-01	-3.29E-01	-9.32E-01	-9.96E-01	6.16E-01	5.75E-01	6.98E-01	-1.25E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	1.14E+00	1.57E+00	2.88E-01	1.48E-01	2.25E+00	4.87E+00	5.30E-01	2.28E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	9.48E-01	5.84E+00	5.33E+00	6.01E+00	6.17E+00	6.32E+00	5.95E+00	6.16E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	3.47E-02	2.52E+00	3.05E+00	3.57E-02	1.61E+00	1.13E-01	2.13E+00	2.47E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	9.92E+00	5.15E+00	5.12E+00	5.01E+00	5.23E+00	5.19E+00	5.33E+00	5.34E+00
d_{head} [Å]	3.15E-01	3.72E-02	3.86E-02	3.47E-02	1.24E-01	6.94E-02	3.85E-02	3.47E-02
a_i	1.01E-01	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.56E-02	7.38E-02
ϵ_{in}	1.00E+00	1.11E+00	1.16E+00	9.74E-01	1.43E+00	1.88E+00	1.00E+00	1.42E+00
α_{ij}^{pol}	2.25E+00	1.46E+00	1.80E+00	1.88E+00	1.50E+00	4.35E-01	8.86E-02	1.54E+00
$w_{\perp}$	7.50E+00	3.10E+00	2.82E+00	-1.57E+00	9.56E-01	-1.70E+00	-7.69E+00	-4.92E-01
$w_{\parallel}$	5.06E+01	8.71E-02	9.04E-02	3.50E-02	6.79E-02	1.81E+01	3.92E-02	1.39E+00

Table 3: Parameters for charged side-chain models interacting with ions.

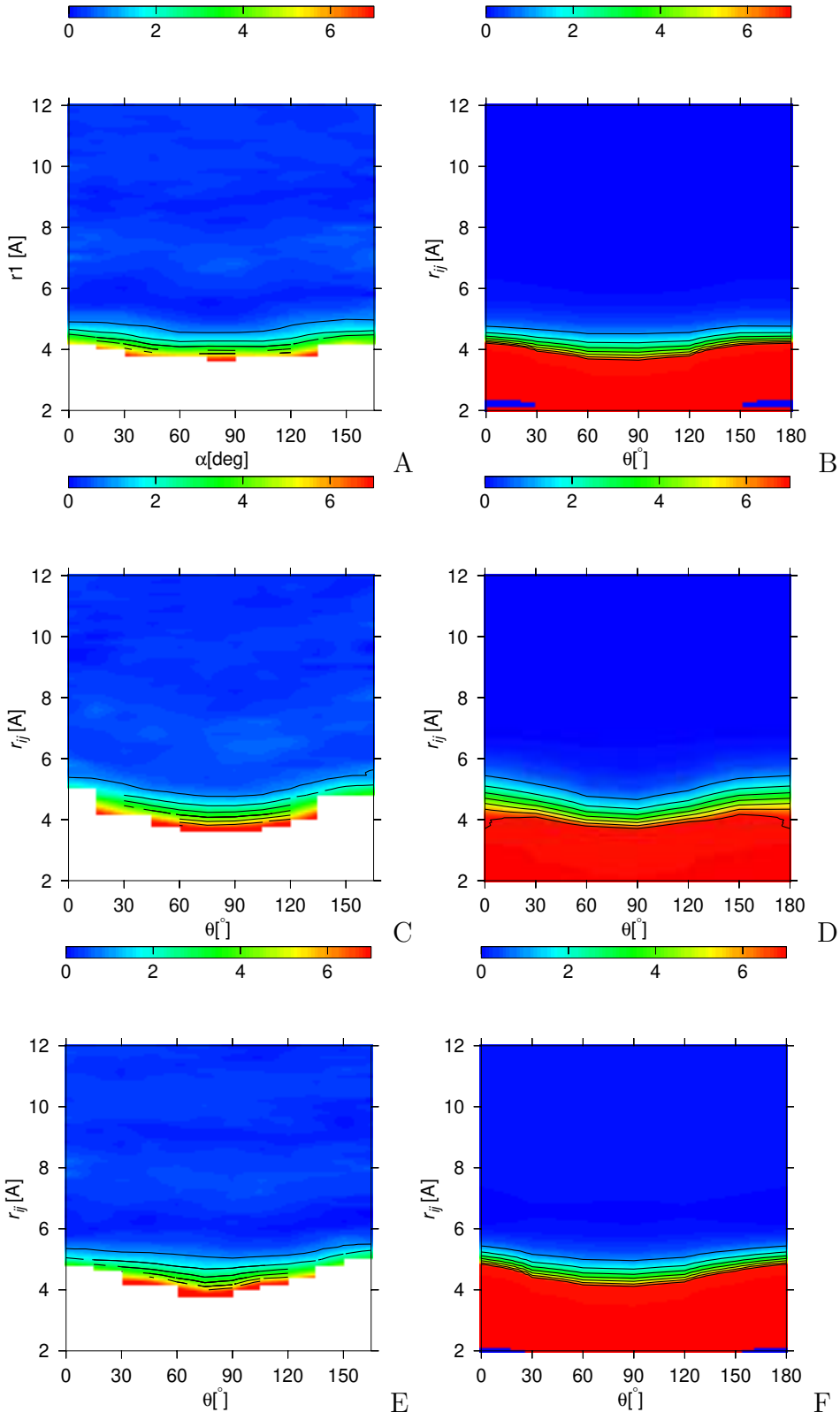
Ca^{2+}				
	asp	glu	lys	arg
ε_{ij}^{0} [kcal/mol]	3.06E+00	7.57E-01	3.53E-01	2.08E+00
σ_{ij}^{0} [Å]	3.99E+00	4.62E+00	1.82E+00	7.53E-01
χ_{ij}	6.99E-01	7.13E-01	9.12E-01	6.81E-01
χ'_{ij}	9.92E-01	9.96E-01	-8.45E-01	1.00E+00
σ [Å]	4.31E+00	5.92E+00	4.33E+00	4.96E+00
$\chi''^{(1)}_{ij}$	-7.26E-01	-9.69E-01	5.17E-01	5.35E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	4.20E+00	3.60E-02	4.30E+00	2.27E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	7.10E+00	5.92E+00	7.34E+00	6.07E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	3.47E-02	6.37E-02	1.11E+00	6.54E-01
$\alpha_{ij}^{(4)}$ [kcal/mol]	5.24E+00	5.26E+00	5.24E+00	5.33E+00
d_{head} [Å]	3.47E-02	3.47E-02	3.47E-02	3.47E-02
a_i	7.82E-02	5.55E-02	6.45E-02	5.55E-02
ϵ_{in}	1.00E+00	1.00E+00	1.00E+00	1.00E+00
κ	1.27E+00	1.60E+00	1.77E+00	1.60E+00
Mg^{2+}				
	asp	glu	lys	arg

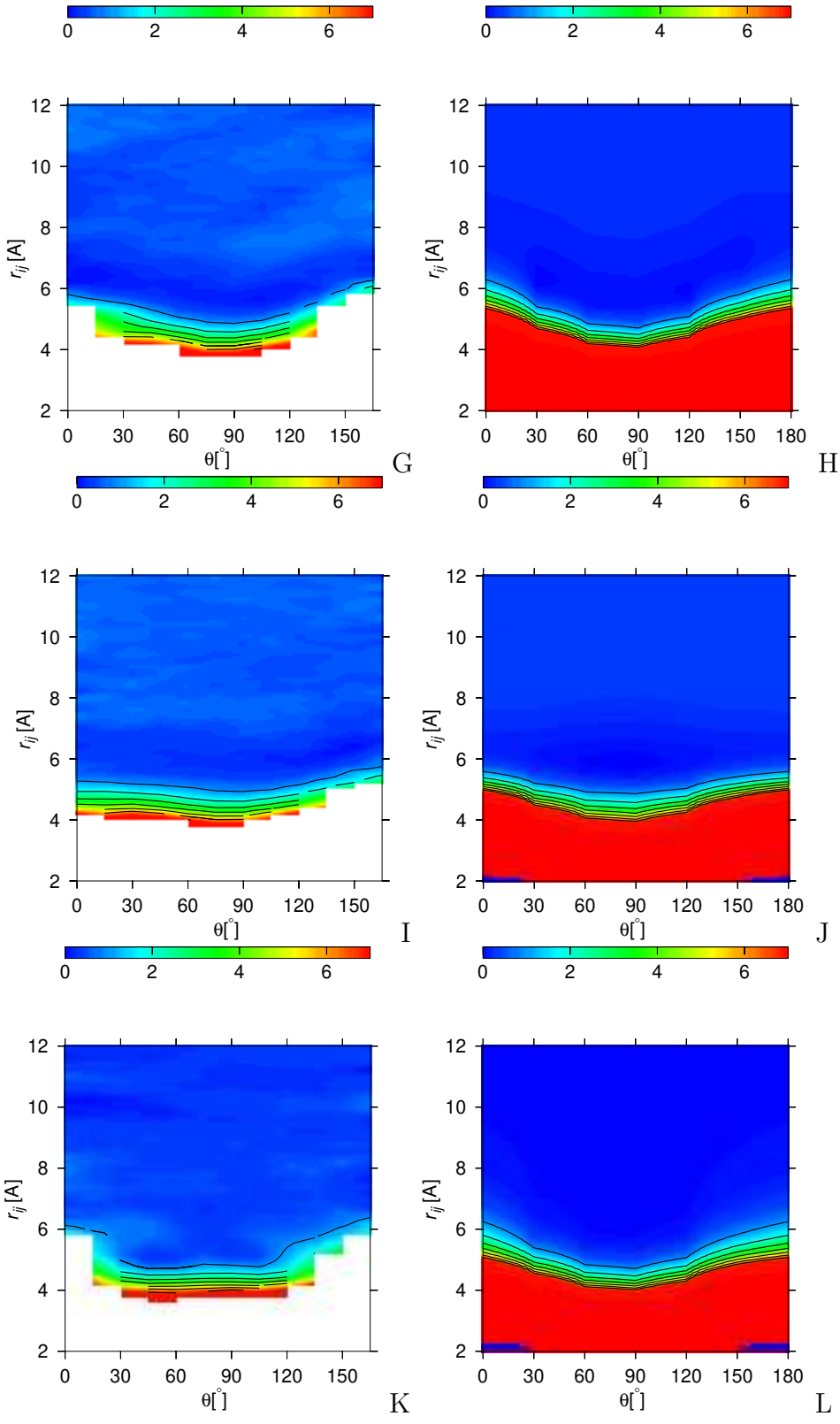
ε_{ij}^{0} [kcal/mol]	8.08E+00	4.42E-02	3.39E+00	3.48E-02
σ_{ij}^{0} [Å]	3.46E+00	5.03E+00	1.99E+00	5.69E+00
χ_{ij}	7.18E-01	4.68E-01	8.76E-01	7.32E-01
χ'_{ij}	7.50E-01	8.85E-01	-9.89E-01	9.96E-01
σ [Å]	4.46E+00	5.39E+00	3.87E+00	7.46E+00
$\chi''^{(1)}_{ij}$	2.41E-01	6.92E-02	5.76E-01	-5.88E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	1.39E+01	3.92E+00	8.97E+00	2.96E-01
$\alpha_{ij}^{(2)}$ [kcal/mol]	1.11E+01	4.04E+00	1.06E+01	7.17E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	1.01E+01	6.66E+00	1.30E+00	4.09E+00
$\alpha_{ij}^{(4)}$ [kcal/mol]	4.69E+00	5.51E+00	4.77E+00	5.10E+00
d_{head} [Å]	3.47E-02	3.47E-02	3.47E-02	3.47E-02
a_i	7.82E-02	5.55E-02	5.55E-02	5.55E-02
ϵ_{in}	1.00E+00	1.00E+00	1.00E+00	1.00E+00
κ	1.37E+00	1.38E+00	2.04E+00	1.73E+00
K^+				
	asp	glu	lys	arg
ε_{ij}^{0} [kcal/mol]	5.43E+00	3.30E+00	3.54E+00	6.92E-01
σ_{ij}^{0} [Å]	3.06E+00	2.93E+00	2.87E+00	2.93E+00
χ_{ij}	7.24E-01	7.27E-01	7.92E-01	6.50E-01

χ'_{ij}	1.00E+00	1.00E+00	8.10E-01	1.00E+00
σ [Å]	4.78E+00	4.58E+00	4.07E+00	3.98E+00
$\chi''^{(1)}_{ij}$	-9.02E-02	3.26E-01	4.72E-01	6.86E-01
$\alpha^{(1)}_{ij}$ [kcal/mol]	1.62E+00	8.27E-01	2.82E+00	2.10E+00
$\alpha^{(2)}_{ij}$ [kcal/mol]	5.98E+00	6.17E+00	6.57E+00	5.92E+00
$\alpha^{(3)}_{ij}$ [kcal/mol]	2.28E+00	5.73E-01	1.69E+00	2.49E+00
$\alpha^{(4)}_{ij}$ [kcal/mol]	5.34E+00	5.35E+00	5.34E+00	5.41E+00
d_{head} [Å]	3.47E-02	3.47E-02	3.47E-02	3.47E-02
a_i	8.69E-02	5.55E-02	5.55E-02	5.55E-02
ϵ_{in}	1.00E+00	1.00E+00	1.00E+00	1.00E+00
κ	1.18E+00	1.37E+00	-8.95E-06	4.93E-02

Na^+				
	asp	glu	lys	arg
ε_{ij}^0 [kcal/mol]	6.55E+00	9.93E+00	3.47E-02	3.47E-02
σ_{ij}^0 [Å]	2.73E+00	2.65E+00	3.88E+00	4.93E+00
χ_{ij}	8.02E-01	2.66E-01	-1.92E-02	6.60E-01
χ'_{ij}	1.00E+00	7.31E-01	1.43E-02	9.10E-01
σ [Å]	4.44E+00	4.26E+00	4.04E+00	2.87E+00
$\chi''^{(1)}_{ij}$	1.34E-01	-7.83E-01	6.33E-01	8.80E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	1.11E+00	1.72E+00	1.52E+00	1.45E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	8.74E+00	5.95E+00	6.23E+00	5.86E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	1.93E+00	3.71E-02	7.96E-01	5.88E-01
$\alpha_{ij}^{(4)}$ [kcal/mol]	5.21E+00	5.38E+00	5.38E+00	5.05E+00
d_{head} [Å]	3.47E-02	3.47E-02	3.47E-02	3.474E-02
a_i	7.82E-02	5.55E-02	5.55E-02	1.01E-01
ϵ_{in}	1.00E+00	1.00E+00	1.00E+00	1.00E+00
κ	5.50E+00	1.61E+00	1.83E+00	1.58E-01
Cl^-				
	asp	glu	lys	arg
ε_{ij}^0 [kcal/mol]	3.28E+00	3.47E-02	3.47E-02	3.47E-02

σ_{ij}^{0} [Å]	3.27E+00	4.55E+00	5.25E+00	4.96E+00
χ_{ij}	7.54E-01	7.28E-01	6.56E-01	6.04E-01
χ'_{ij}	1.00E+00	9.95E-01	9.68E-01	-6.77E-01
σ [Å]	4.44E+00	4.42E+00	1.36E+00	3.38E+00
$\chi_{ij}^{\prime\prime(1)}$	2.52E-01	4.43E-01	6.82E-01	6.51E-01
$\alpha_{ij}^{(1)}$ [kcal/mol]	1.65E+00	8.20E-01	3.00E+00	1.70E+00
$\alpha_{ij}^{(2)}$ [kcal/mol]	6.16E+00	5.99E+00	8.32E+00	5.91E+00
$\alpha_{ij}^{(3)}$ [kcal/mol]	2.96E-01	3.48E-02	2.81E+00	4.60E-01
$\alpha_{ij}^{(4)}$ [kcal/mol]	5.34E+00	5.37E+00	4.46E+00	6.10E+00
d_{head} [Å]	3.47E-02	3.47E-02	3.47E-02	3.47E-02
a_i	7.82E-02	5.55E-02	1.01E-01	1.11E+00
ϵ_{in}	1.00E+00	1.00E+00	1.00E+00	1.00E+00
κ	-4.75E-03	1.57E+00	8.54E+00	3.42E-01


0 2 4 6
12
10
8
6
4
2
r1 [A]
0 30 60 90 120 150
α[deg]
A
0 2 4 6
0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
C
0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
D
0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
E
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
F


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
H
I
J
K
L

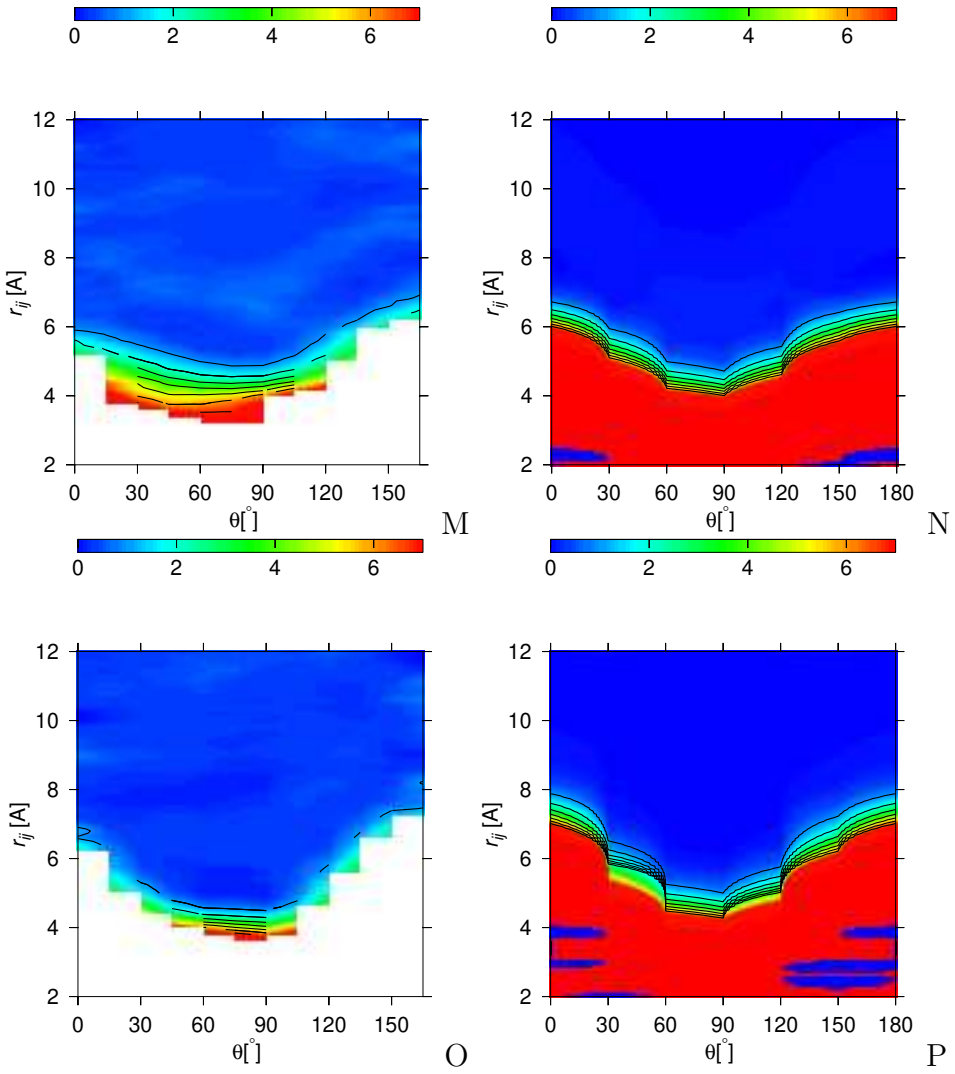
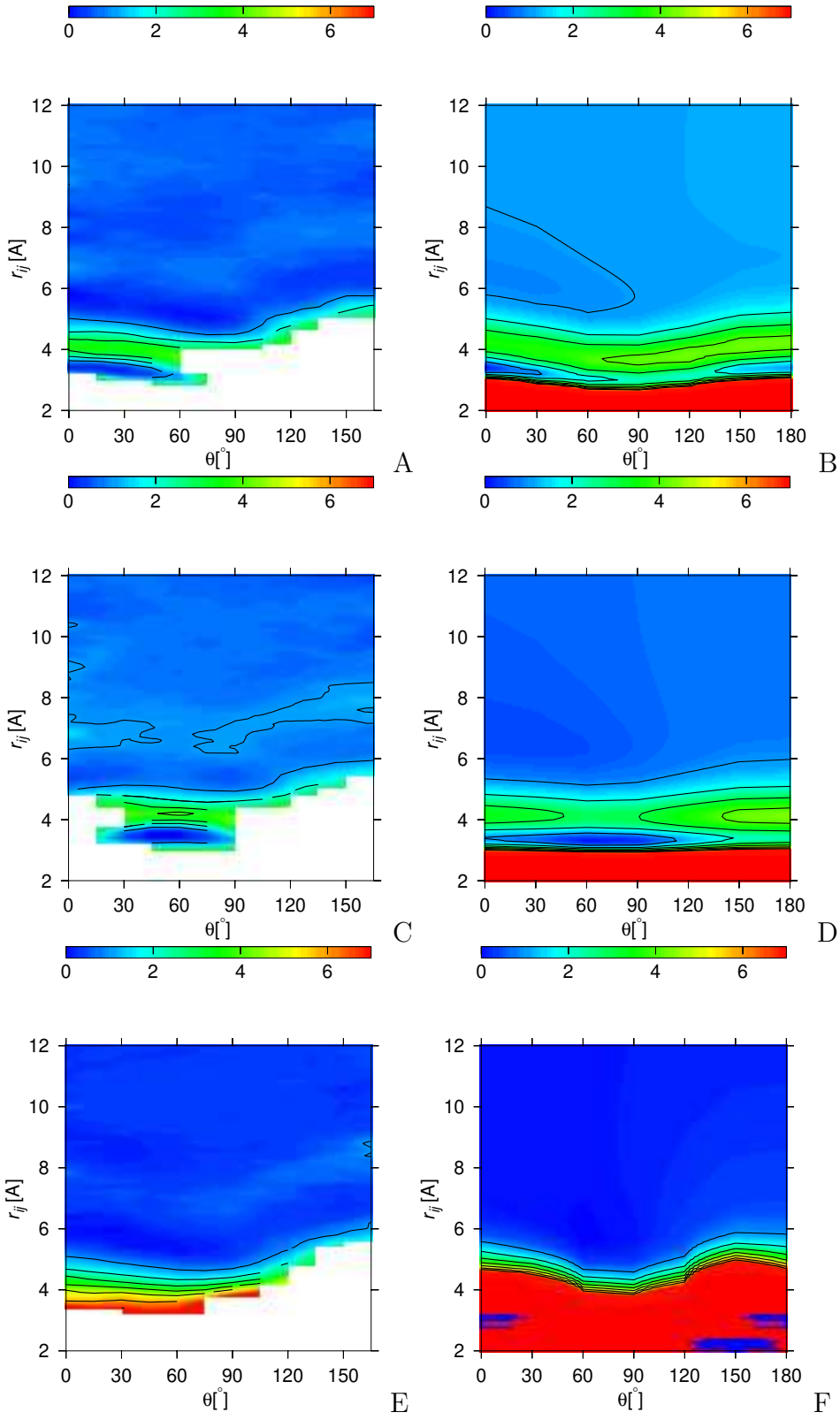
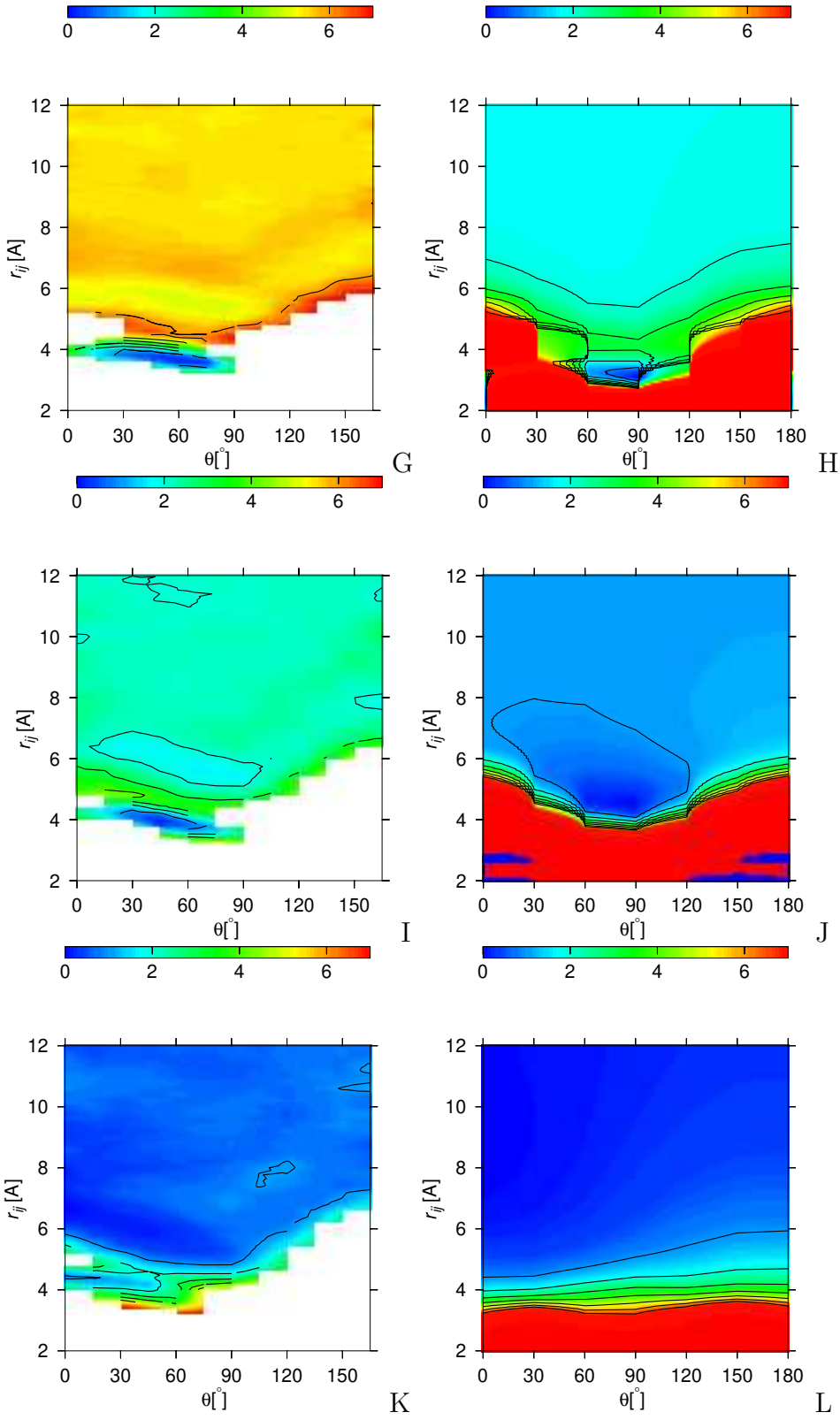


Figure 1: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Ca^{2+} interacting with hydrophobic side-chain models: alanine (A) and (B), proline (C) and (D), valine (E) and (F), leucine (G) and (H), isoleucine (I) and (J), phenylalanine (K) and (L), methionine (M) and (N), tryptophan (O) and (P).


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
0 2 4 6
C
D
E
F


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
0 2 4 6
I
J
K
L

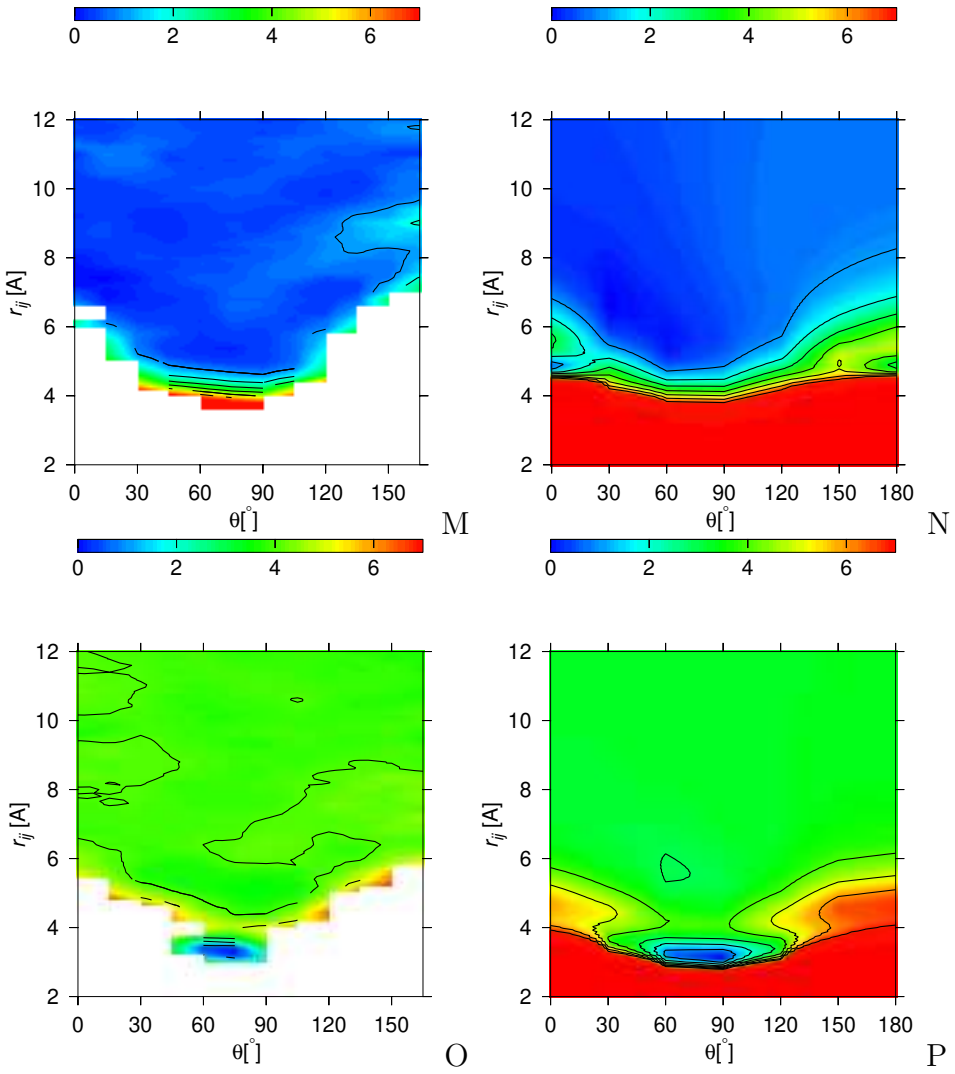
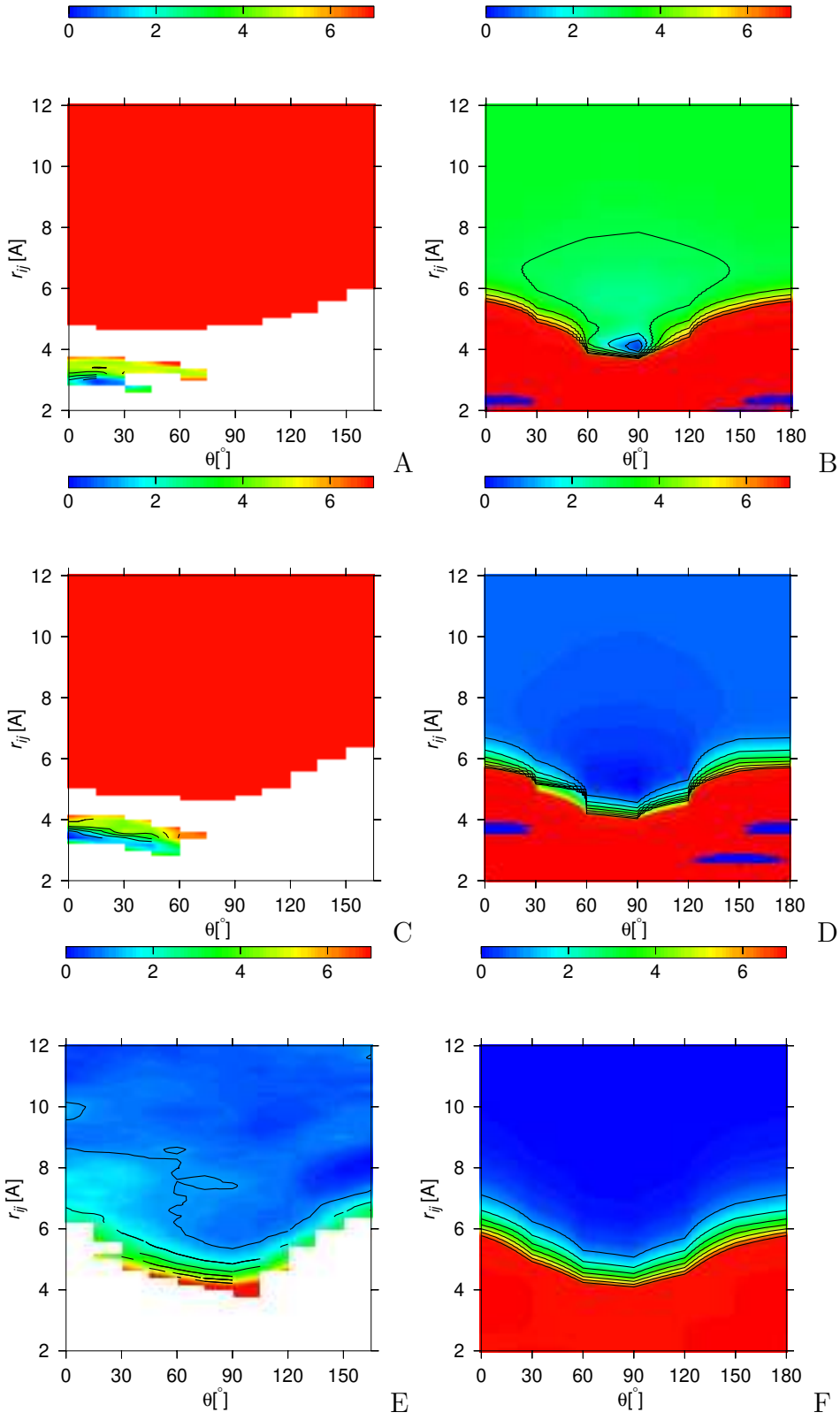


Figure 2: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Ca^{2+} interacting with polar side-chain models: serine (A) and (B), threonine (C) and (D), cysteine (E) and (F), asparagine (G) and (H), glutamine (I) and (J), histidine (K) and (L), tyrosine (M) and (N), and peptide group (O) and (P).


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 30 60 90 120 150 180
θ[°]
B
C
D
E
F

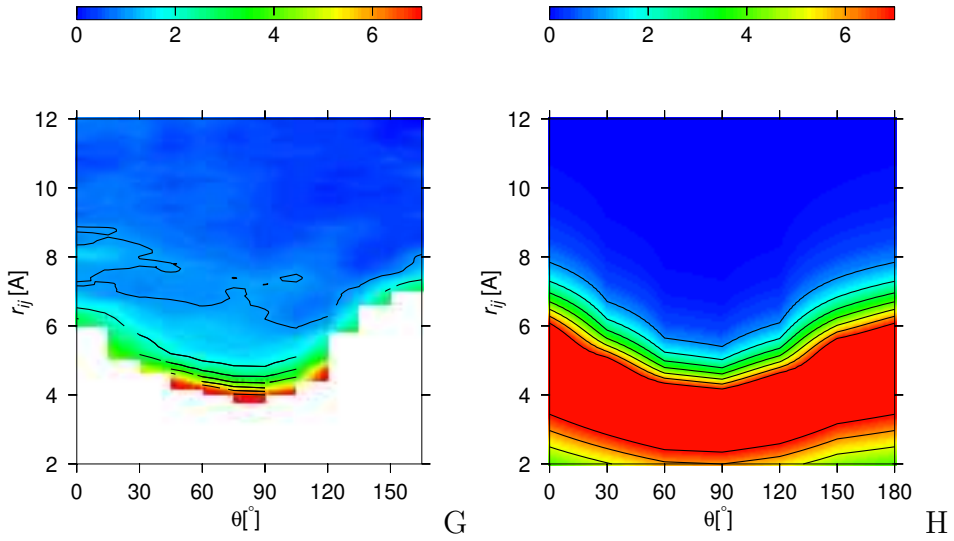
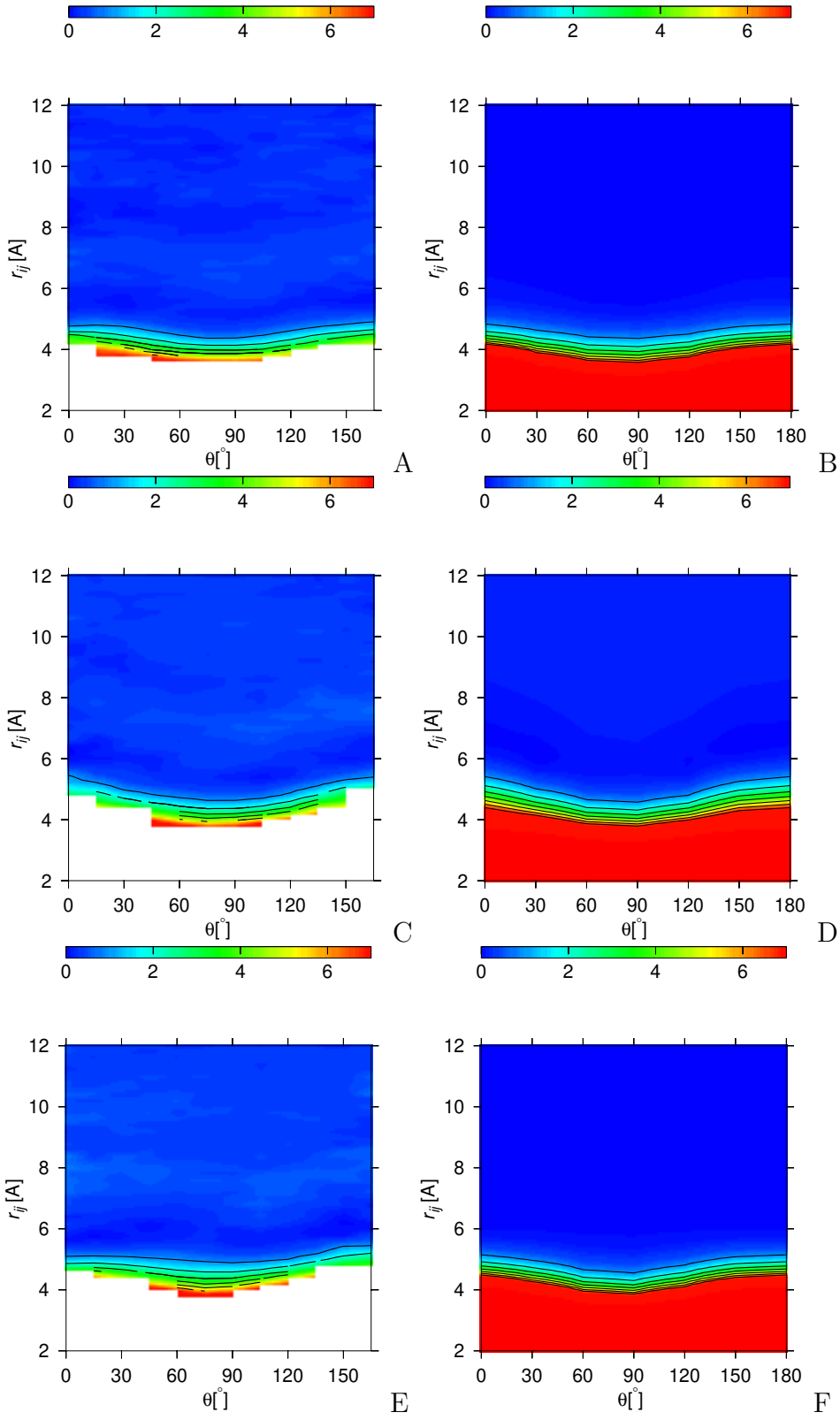
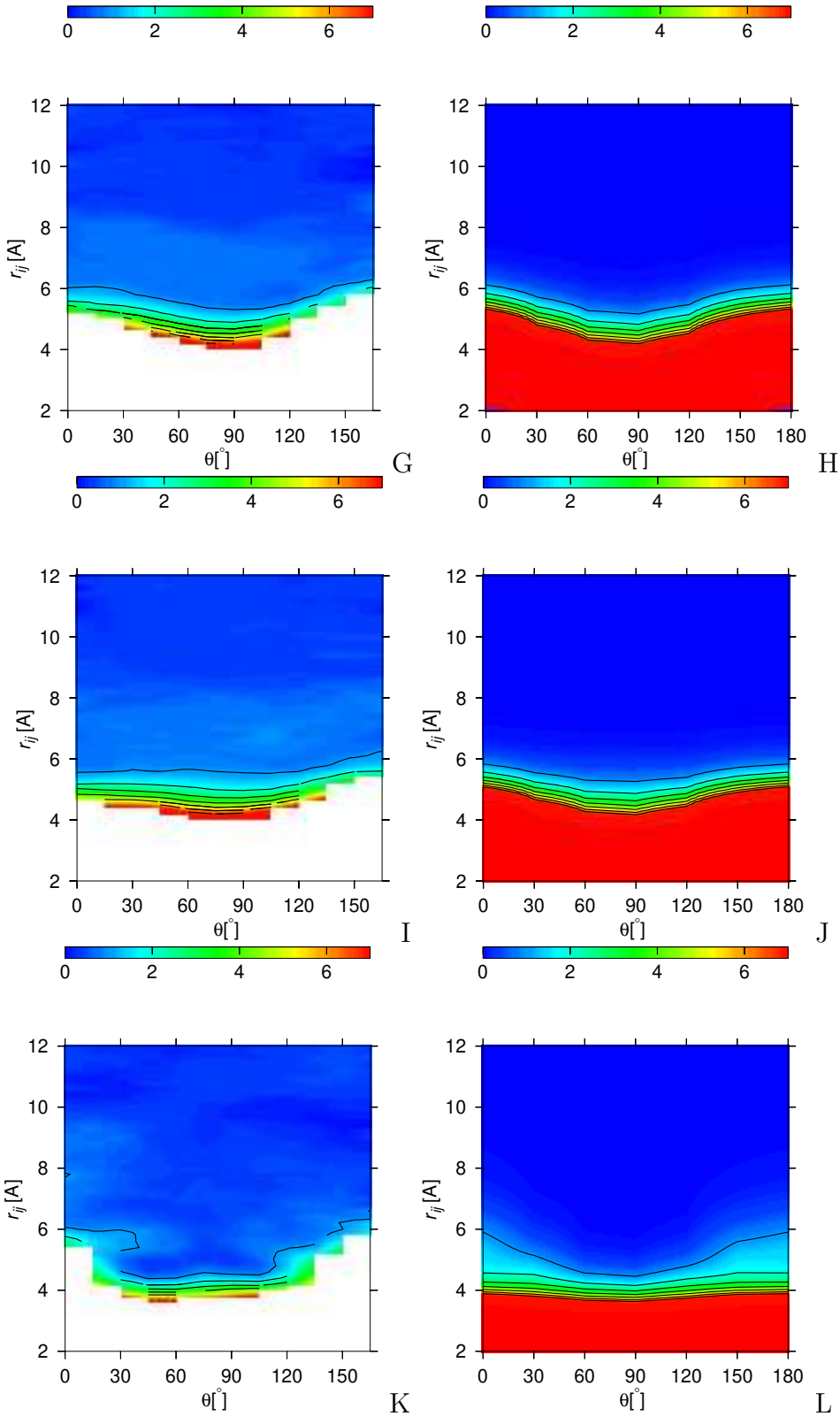


Figure 3: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Ca^{2+} interacting with charged side-chain models: aspartic acid (A) and (B), glutamic acid (C) and (D), lysine (E) and (F), arginine (G) and (H).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
C
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
D
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
E
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
F


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
0 2 4 6
I
J
K
L

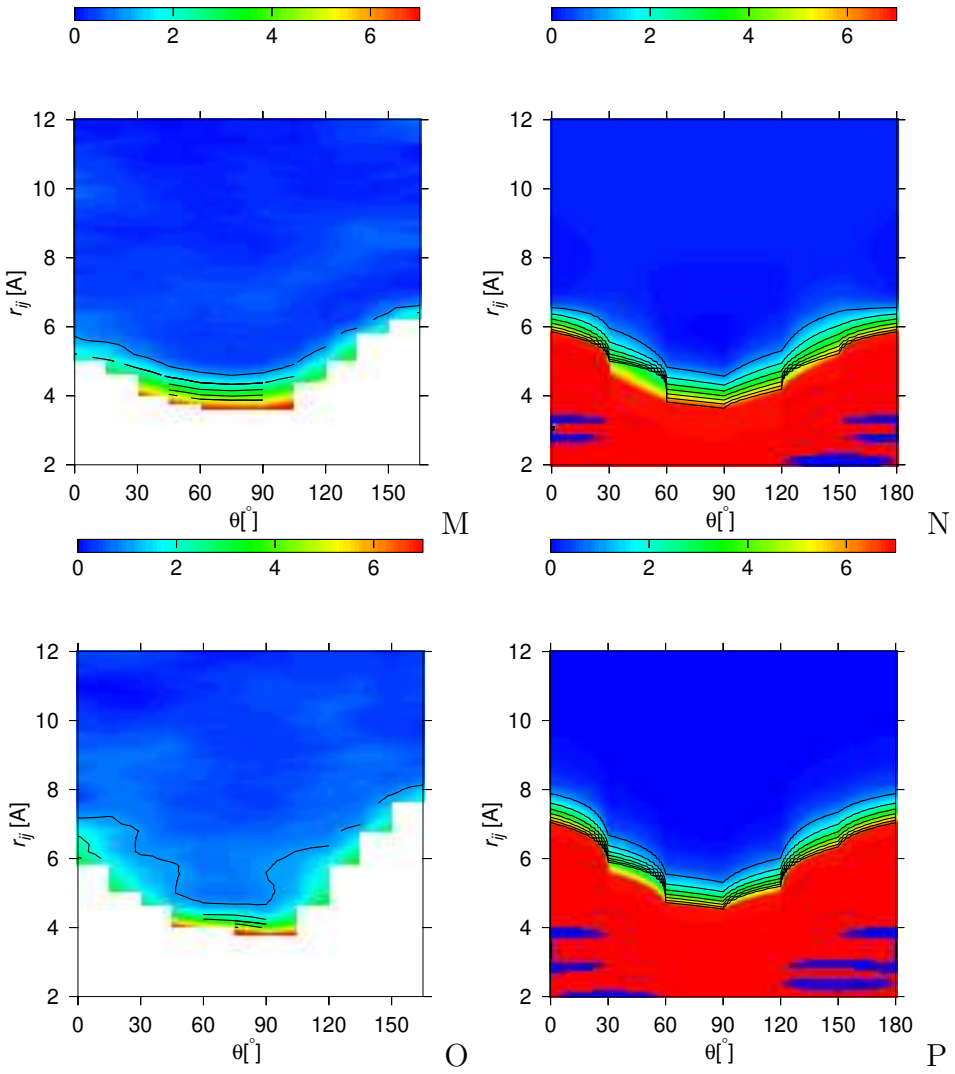
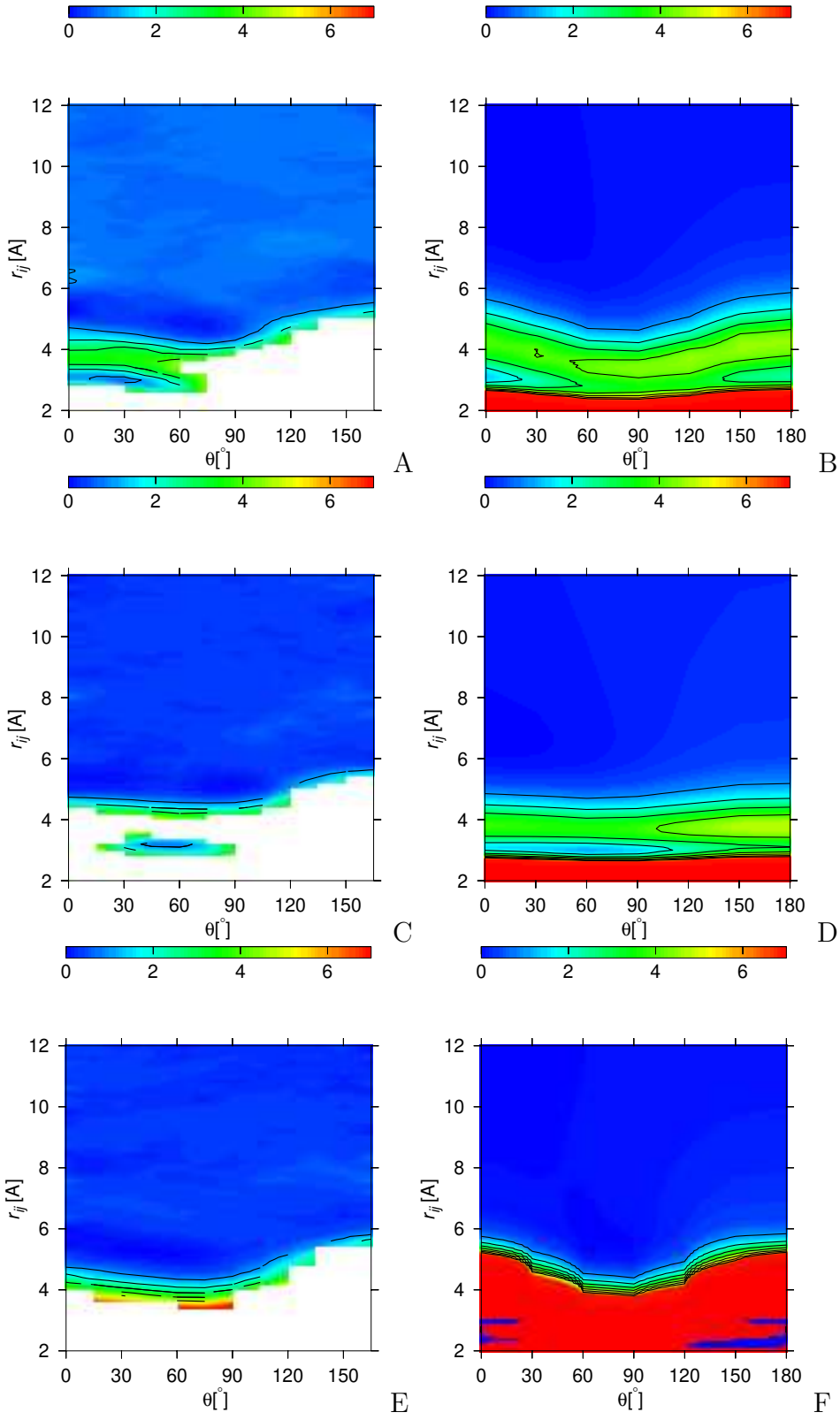
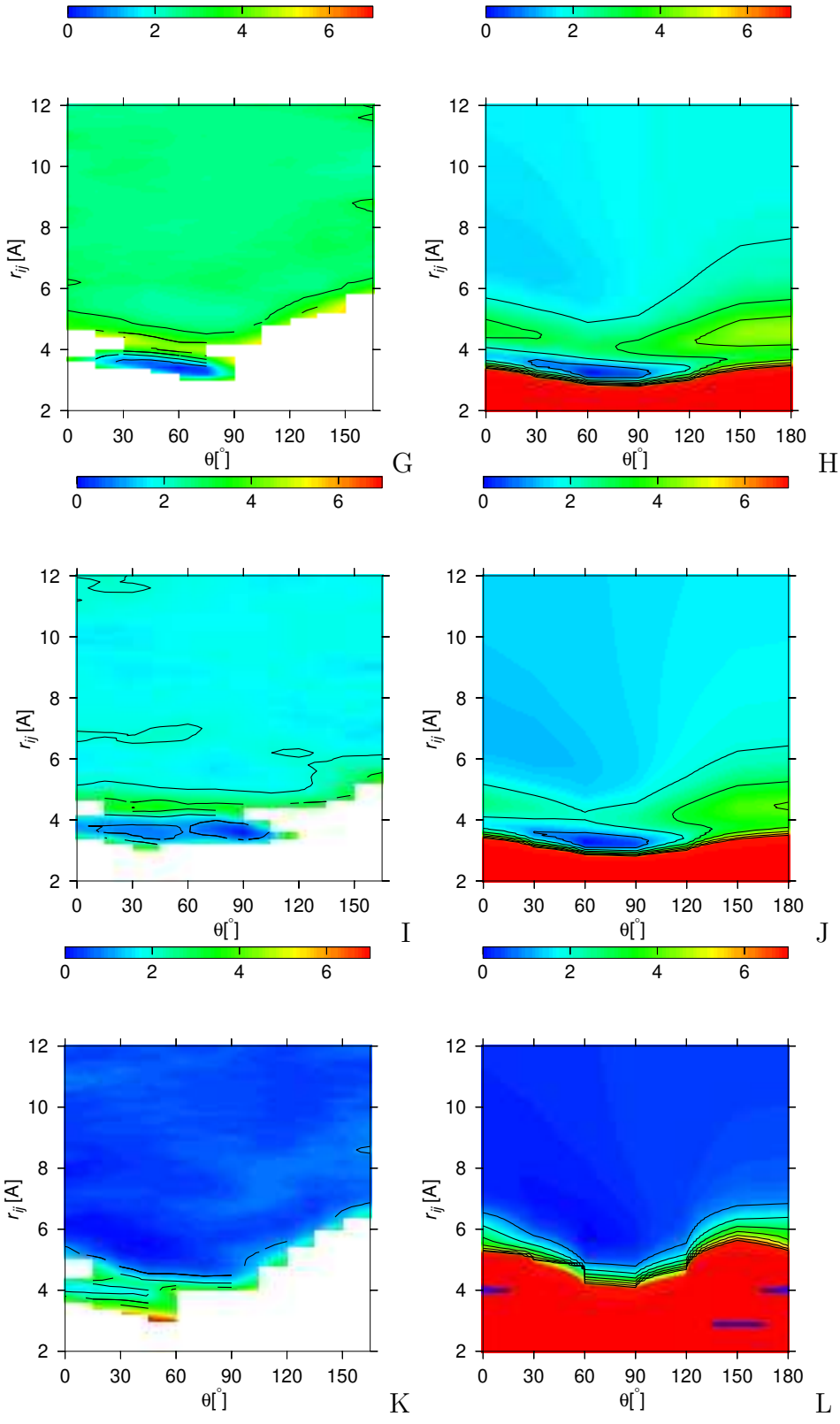


Figure 4: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Mg^{2+} interacting with hydrophobic side-chain models: alanine (A) and (B), proline (C) and (D), valine (E) and (F), leucine (G) and (H), isoleucine (I) and (J), phenylalanine (K) and (L), methionine (M) and (N), tryptophan (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
C
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
D
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
E
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
F


0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 2 4 6
0 2 4 6
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
I
J
K
L

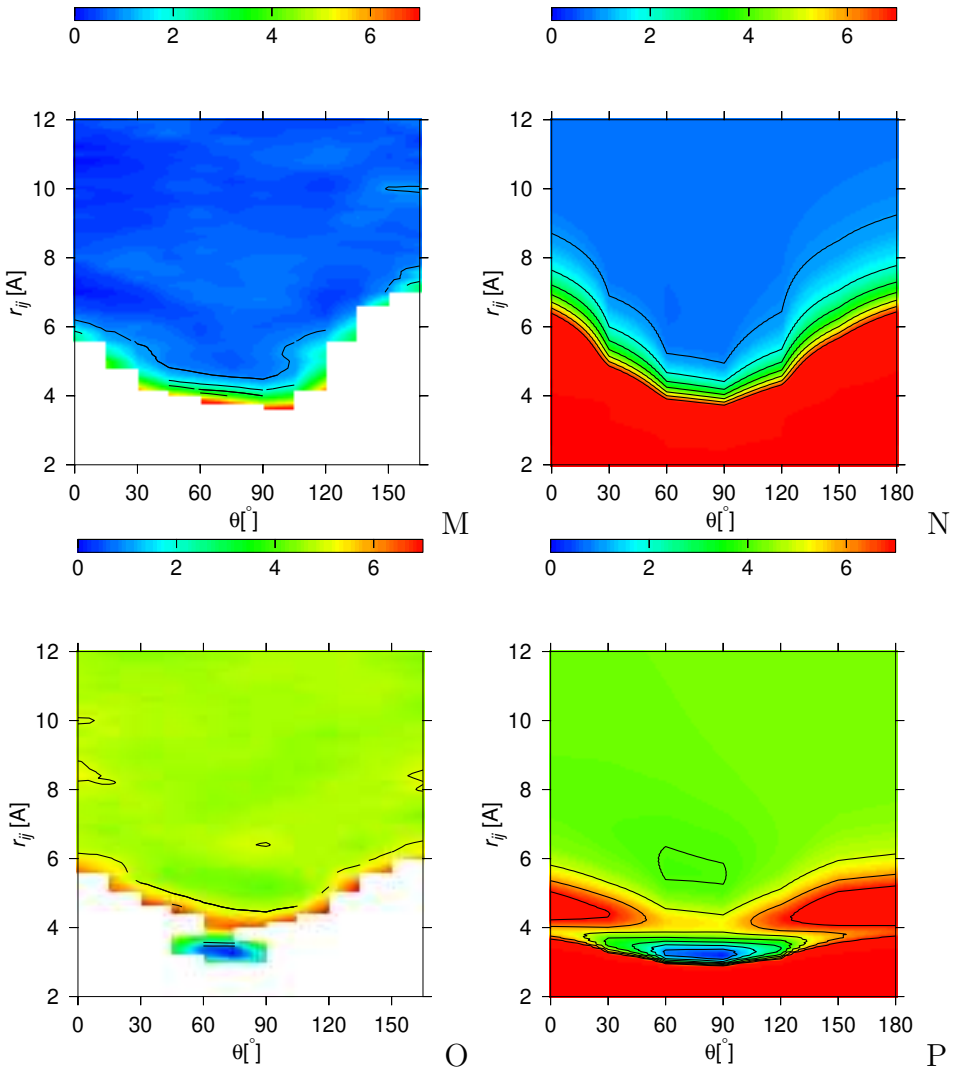
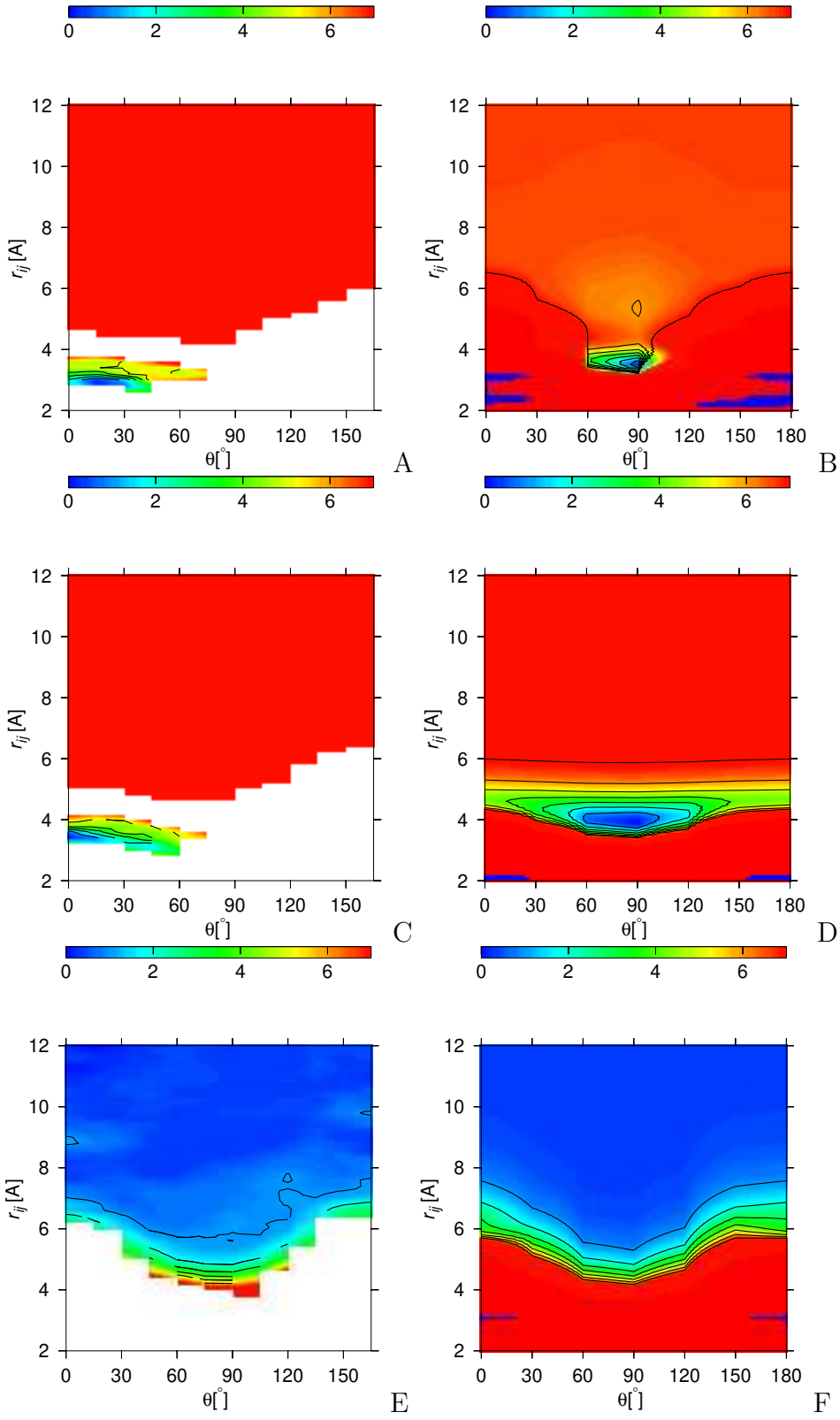


Figure 5: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Mg^{2+} interacting with polar side-chain models: serine (A) and (B), threonine (C) and (D), cysteine (E) and (F), asparagine (G) and (H), glutamine (I) and (J), histidine (K) and (L), tyrosine (M) and (N), and peptide group (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 30 60 90 120 150 180
θ[°]
B
C
D
E
F

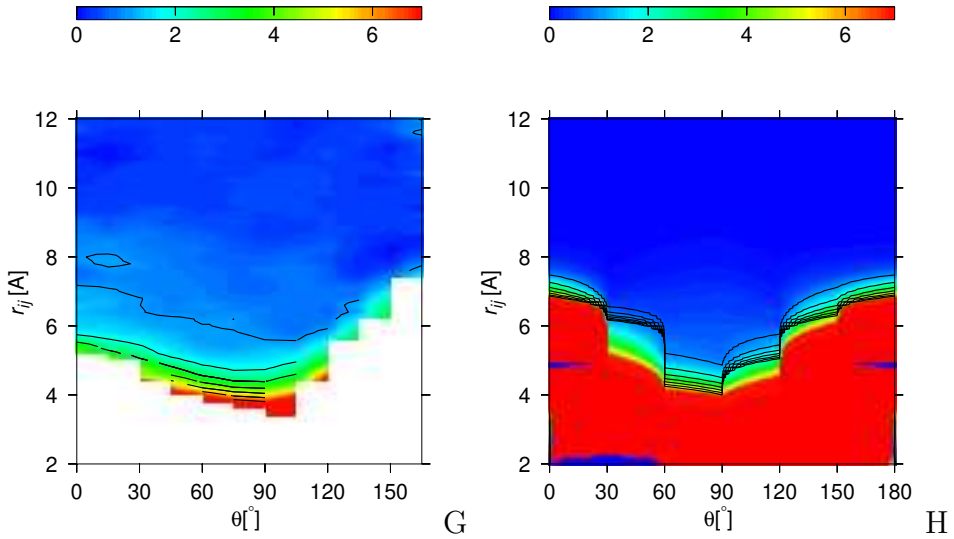
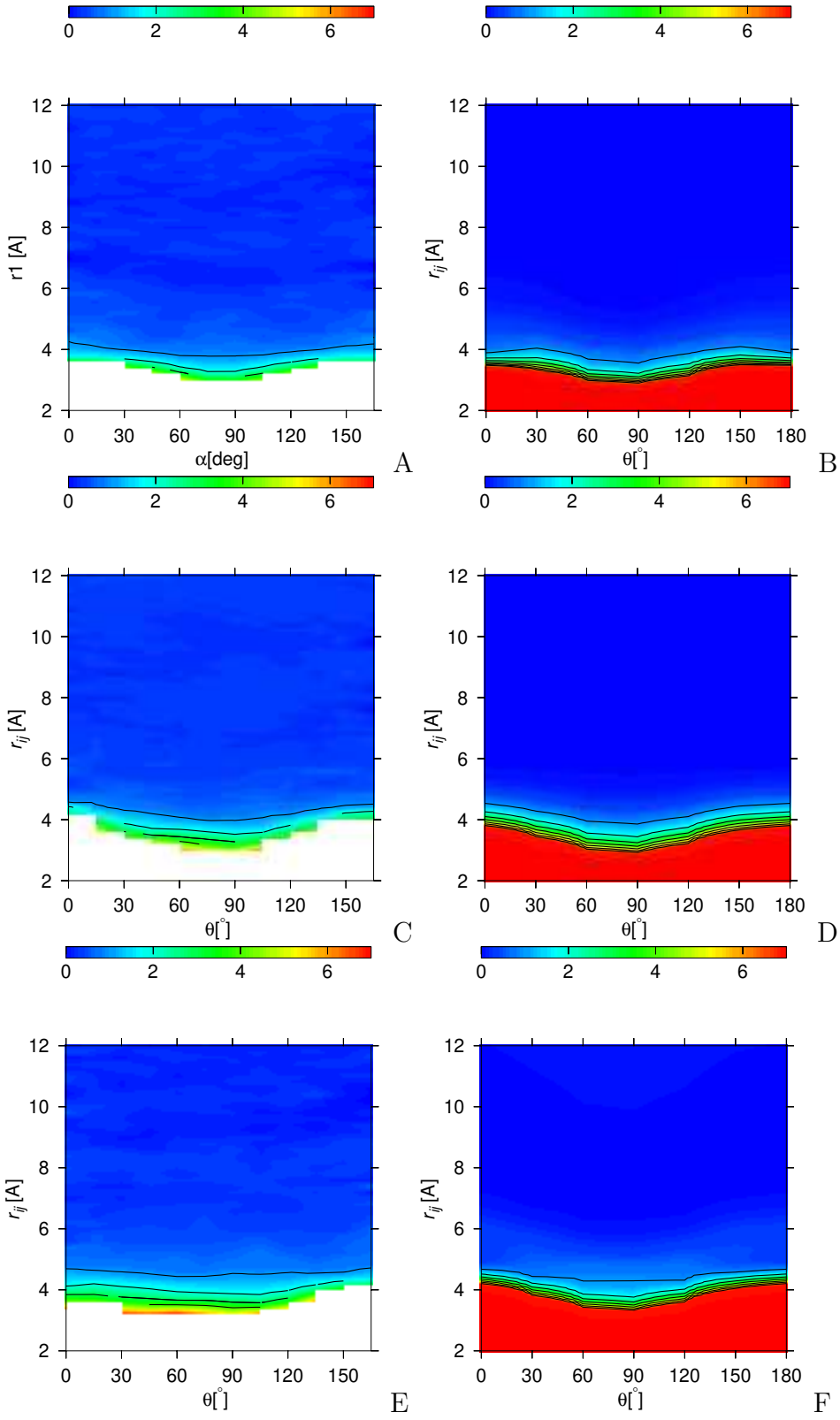
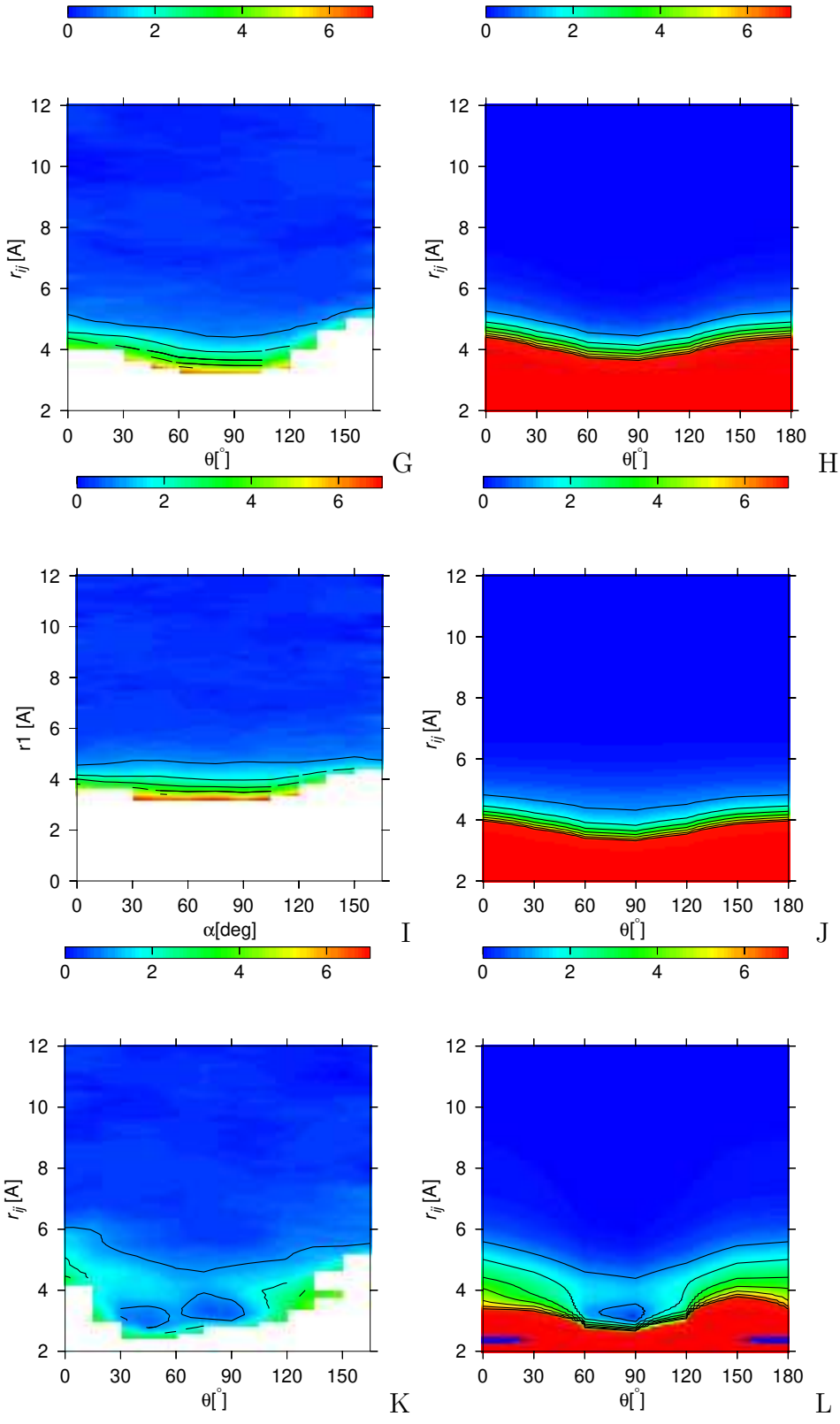


Figure 6: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Mg^{2+} interacting with charged side-chain models: aspartic acid (A) and (B), glutamic acid (C) and (D), lysine (E) and (F), arginine (G) and (H).


0 2 4 6
r1 [A]
α[deg]
A
r_{ij} [A]
θ[°]
B
C
D
E
F


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
0 2 4 6
r1 [A]
0 30 60 90 120 150
α[deg]
I
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
J
0 2 4 6
0 2 4 6
r_{ij} [A]
0 30 60 90 120 150
θ[°]
K
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
L

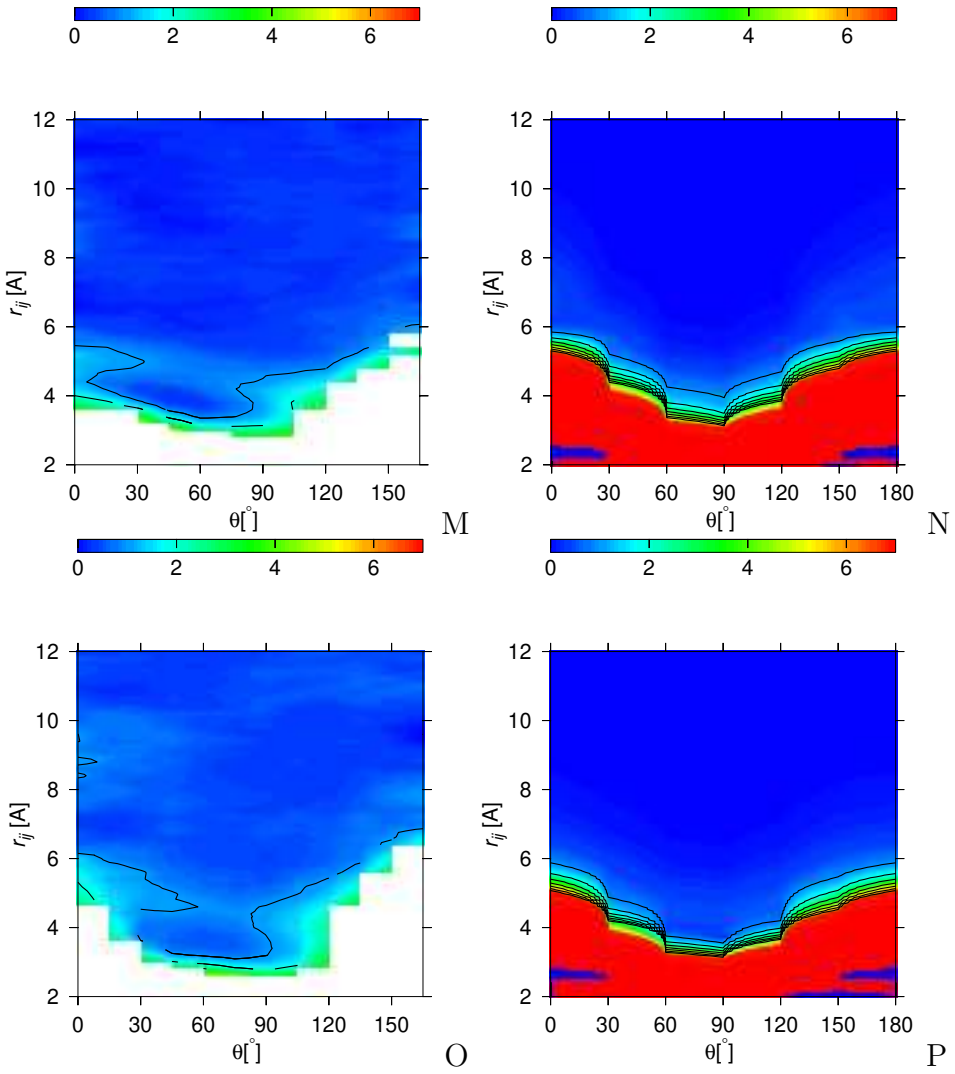
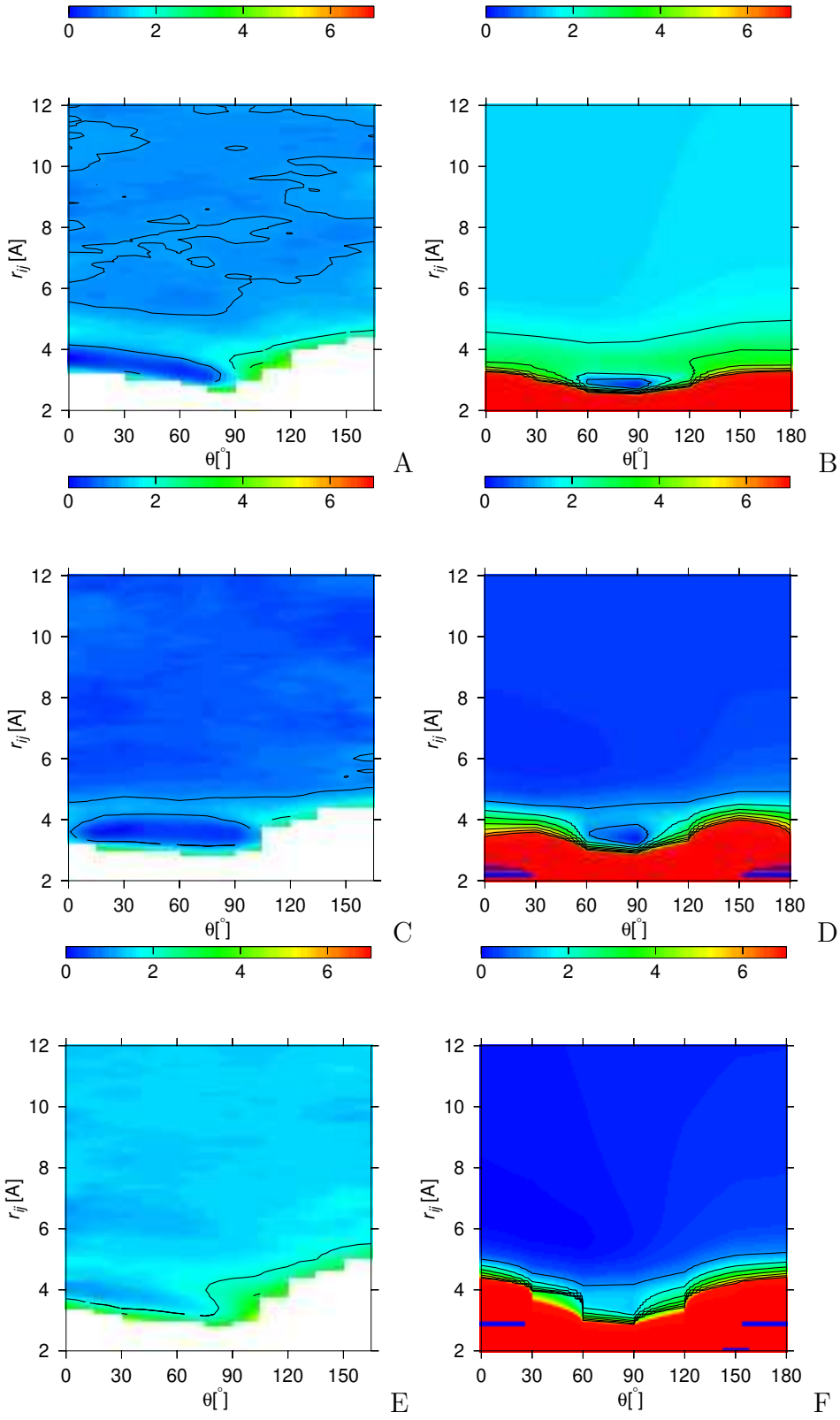
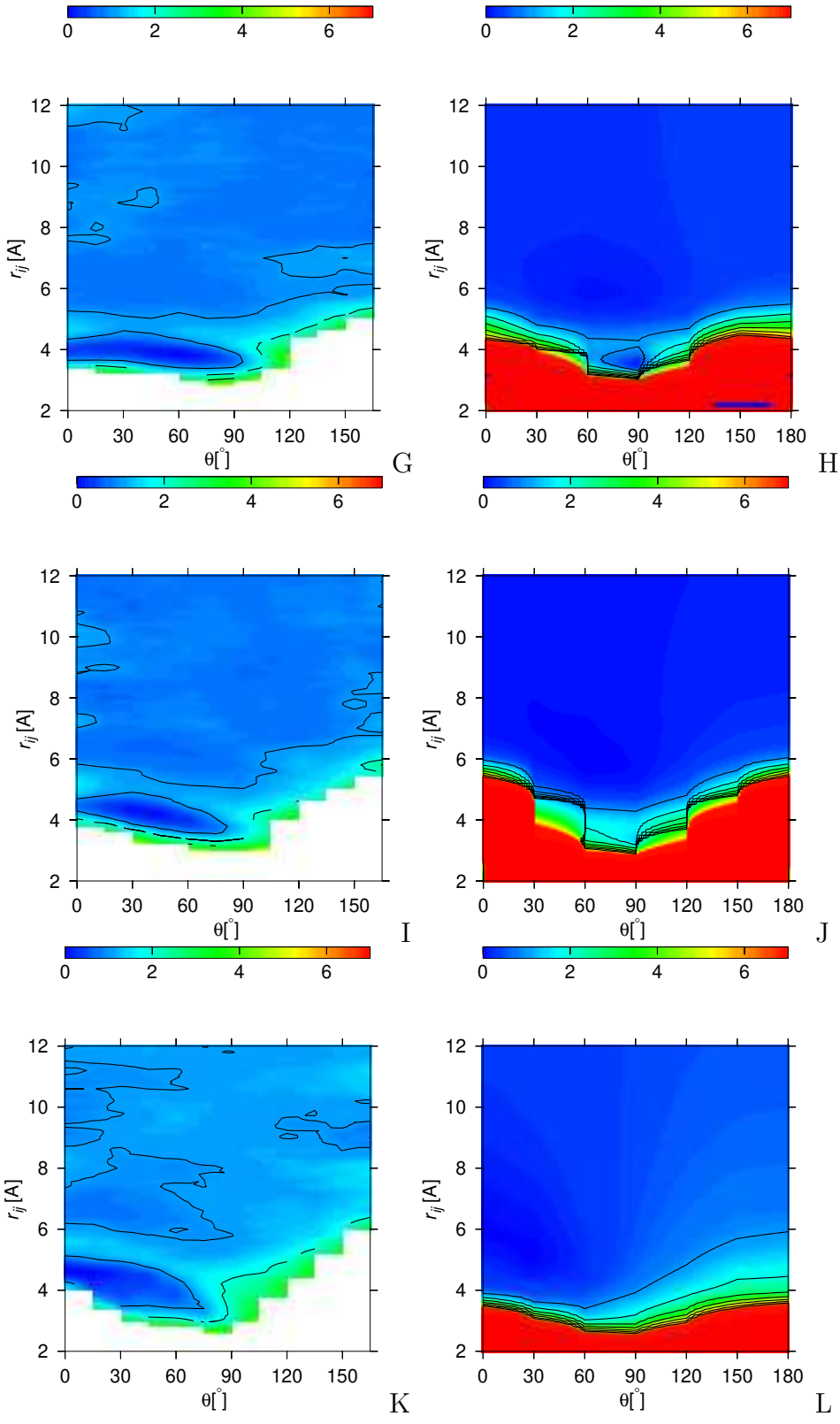


Figure 7: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for K^+ interacting with hydrophobic side-chain models: alanine (A) and (B), proline (C) and (D), valine (E) and (F), leucine (G) and (H), isoleucine (I) and (J), phenylalanine (K) and (L), methionine (M) and (N), tryptophan (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 30 60 90 120 150 180
B
C
D
E
F


0 2 4 6
12
10
8
6
4
2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 2 4 6
0 2 4 6
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
I
J
K
L

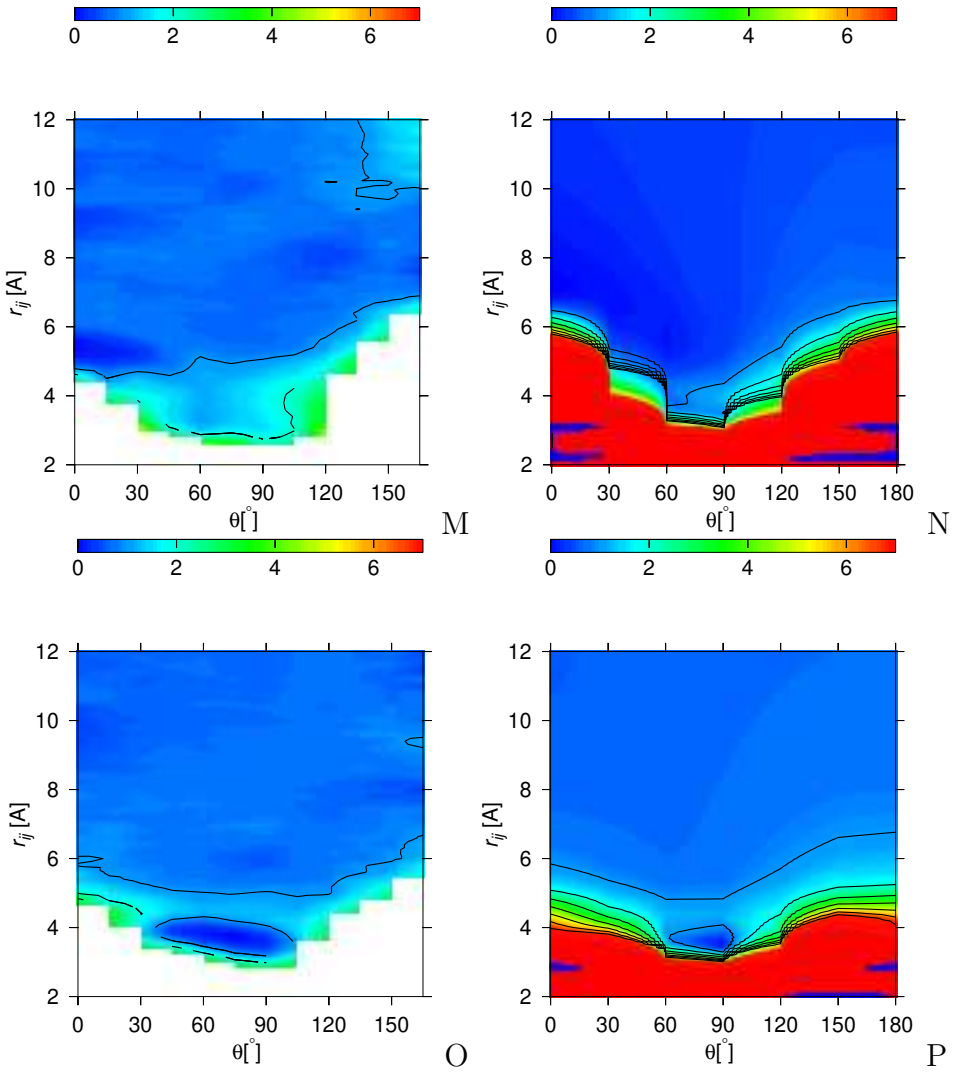
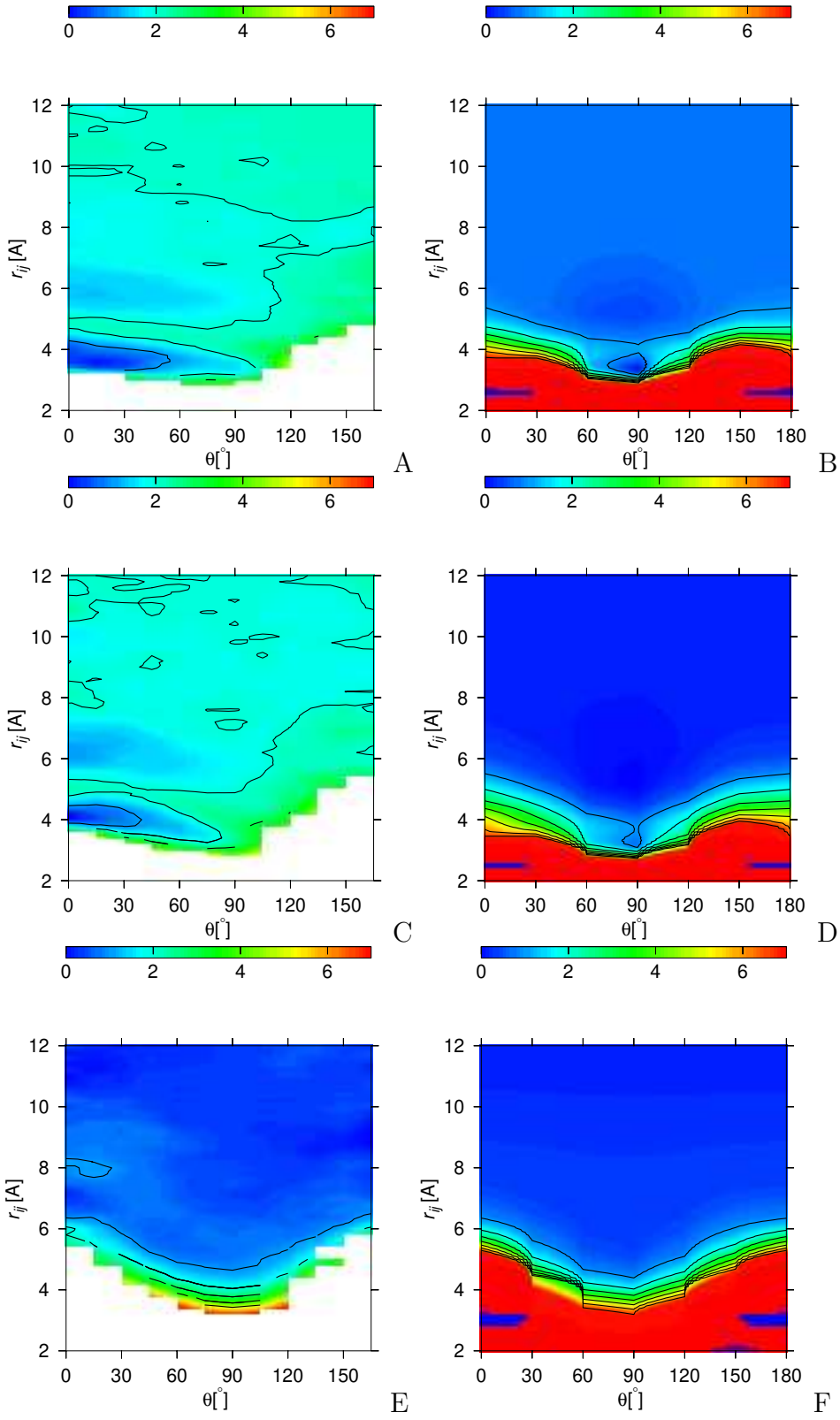


Figure 8: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for K^+ interacting with polar side-chain models: serine (A) and (B), threonine (C) and (D), cysteine (E) and (F), asparagine (G) and (H), glutamine (I) and (J), histidine (K) and (L), tyrosine (M) and (N), and peptide group (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
C
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
D
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
E
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
F

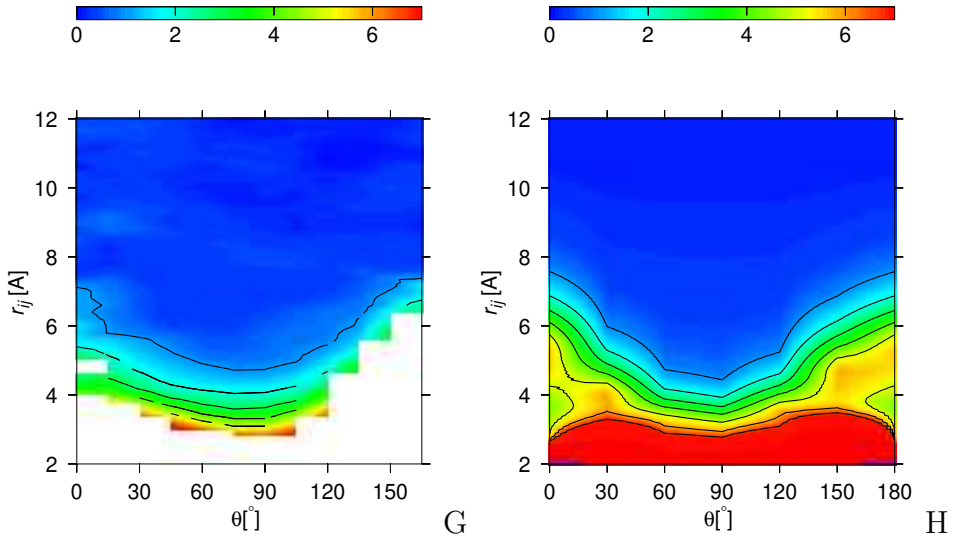
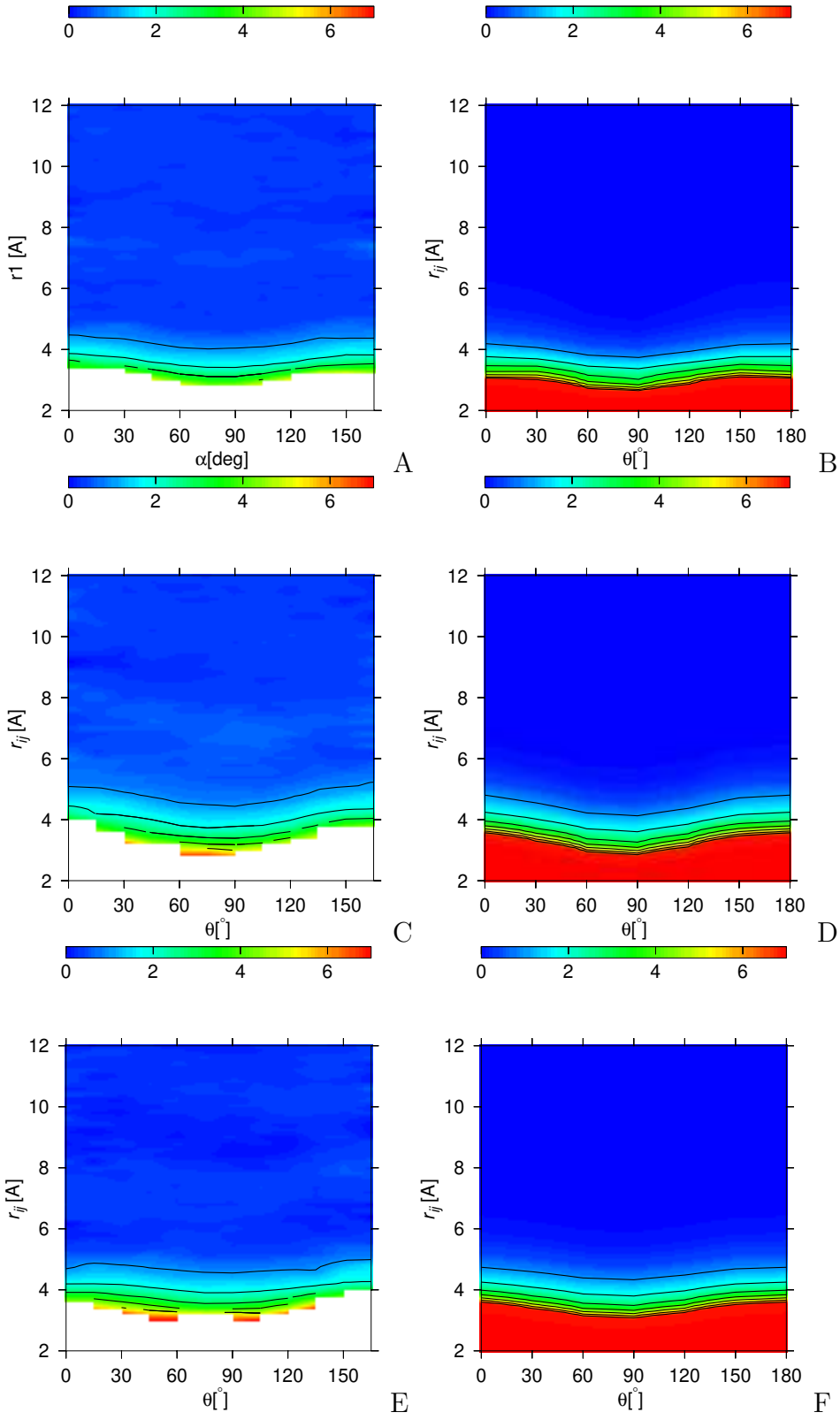
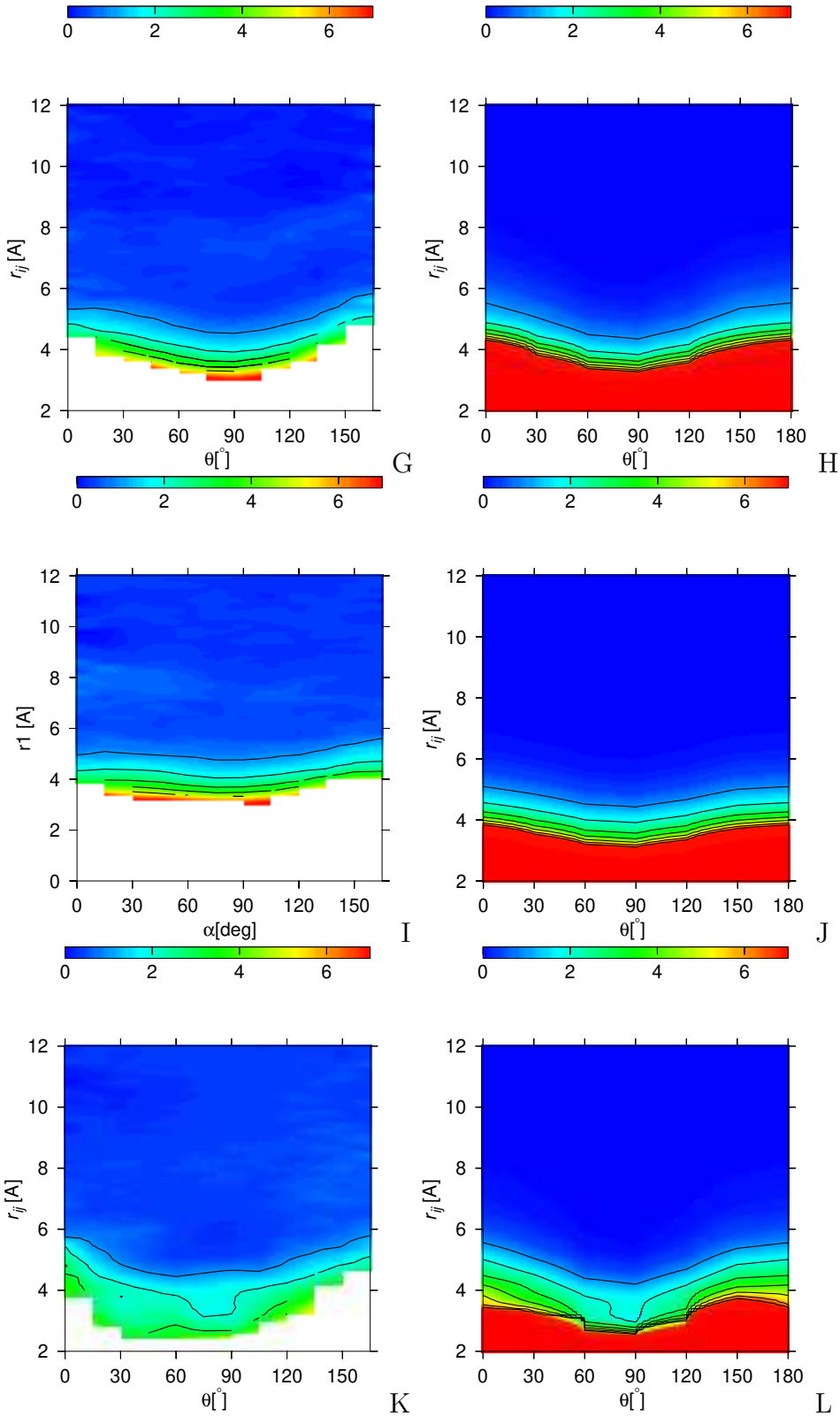


Figure 9: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for K^+ interacting with charged side-chain models: aspartic acid (A) and (B), glutamic acid (C) and (D), lysine (E) and (F), arginine (G) and (H).


0 2 4 6
r1 [A]
α[deg]
A
r_{ij} [A]
θ[°]
B
C
D
E
F


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
12 10 8 6 4 2 0
r1 [A]
0 30 60 90 120 150
α[deg]
I
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
J
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
K
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
L

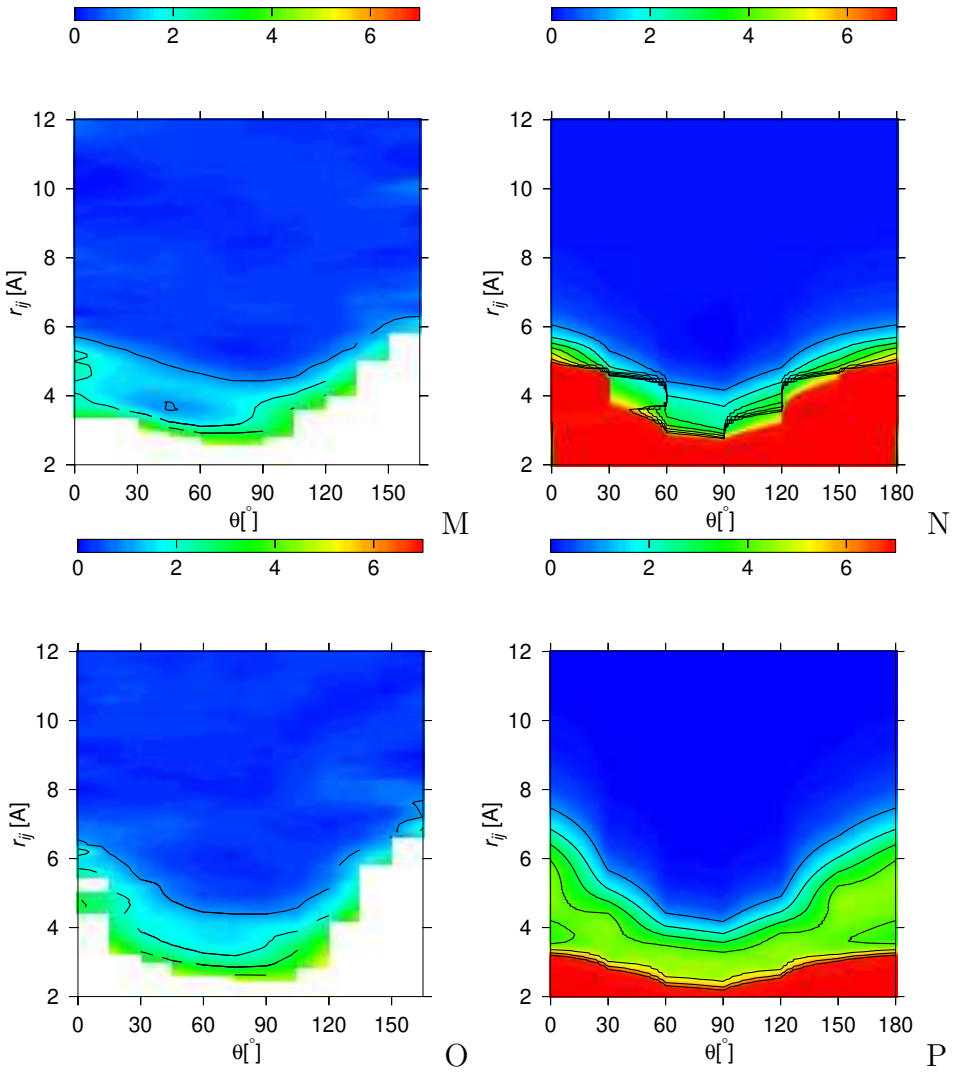
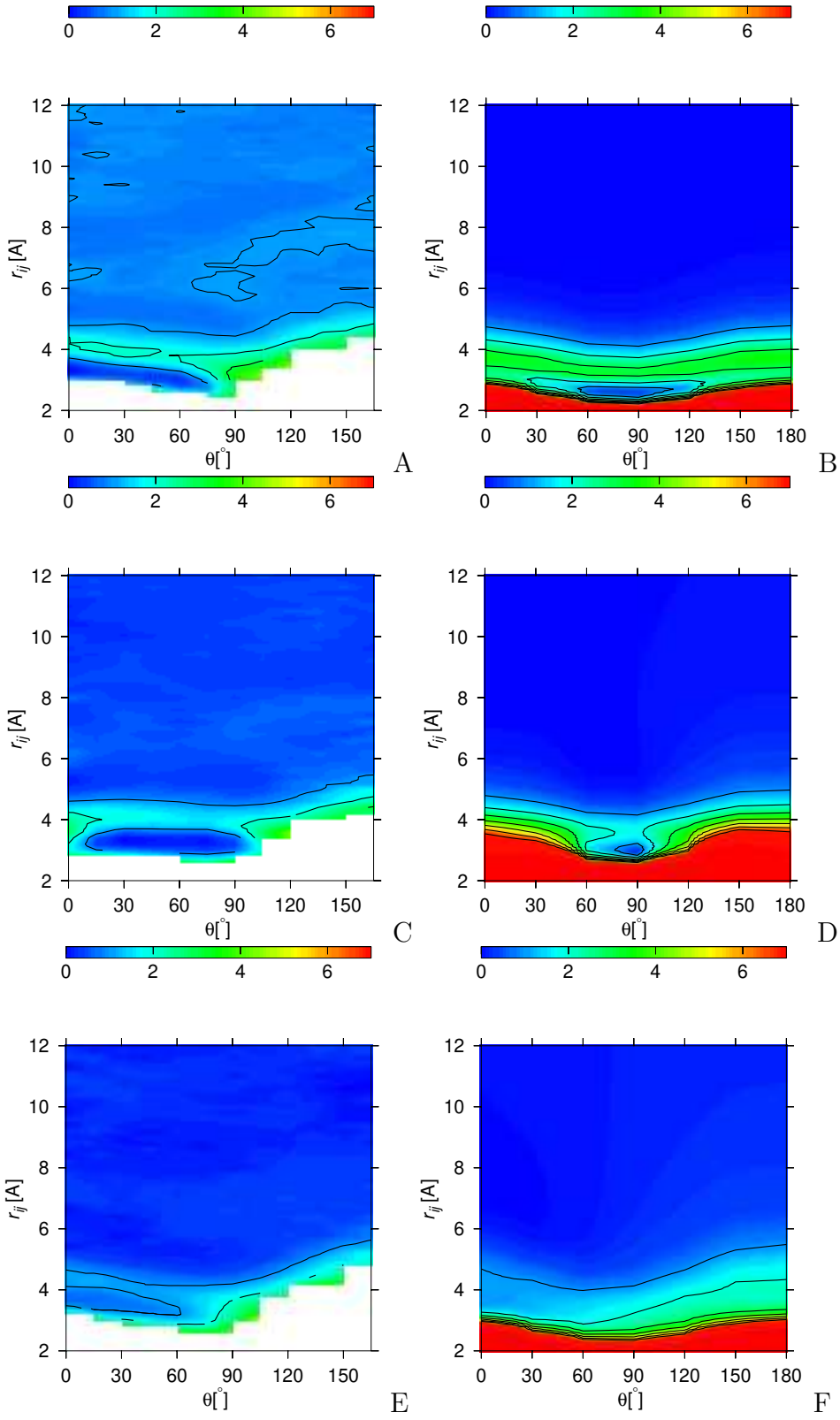
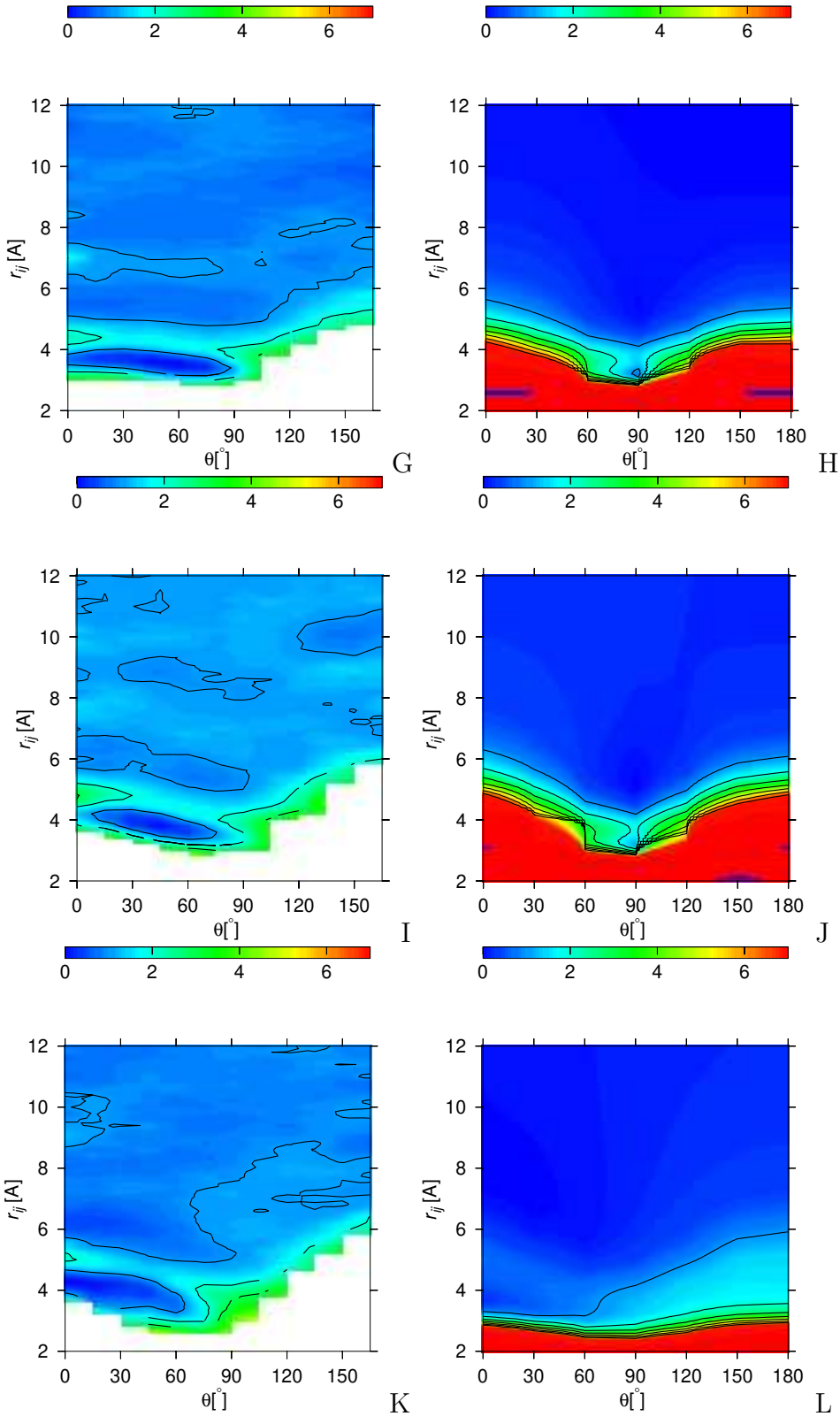


Figure 10: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Na^+ interacting with hydrophobic side-chain models: alanine (A) and (B), proline (C) and (D), valine (E) and (F), leucine (G) and (H), isoleucine (I) and (J), phenylalanine (K) and (L), methionine (M) and (N), tryptophan (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 30 60 90 120 150 180
B
C
D
E
F


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
0 2 4 6
I
J
K
L

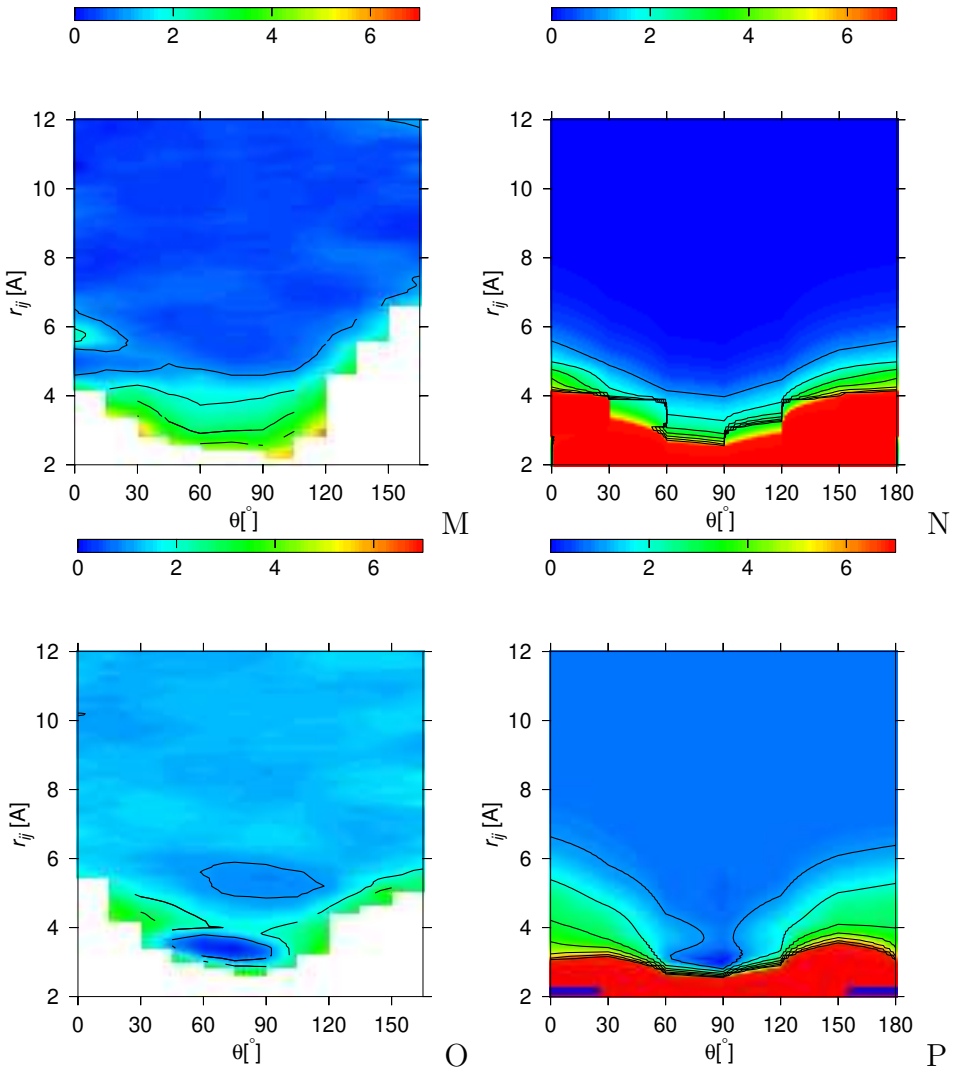
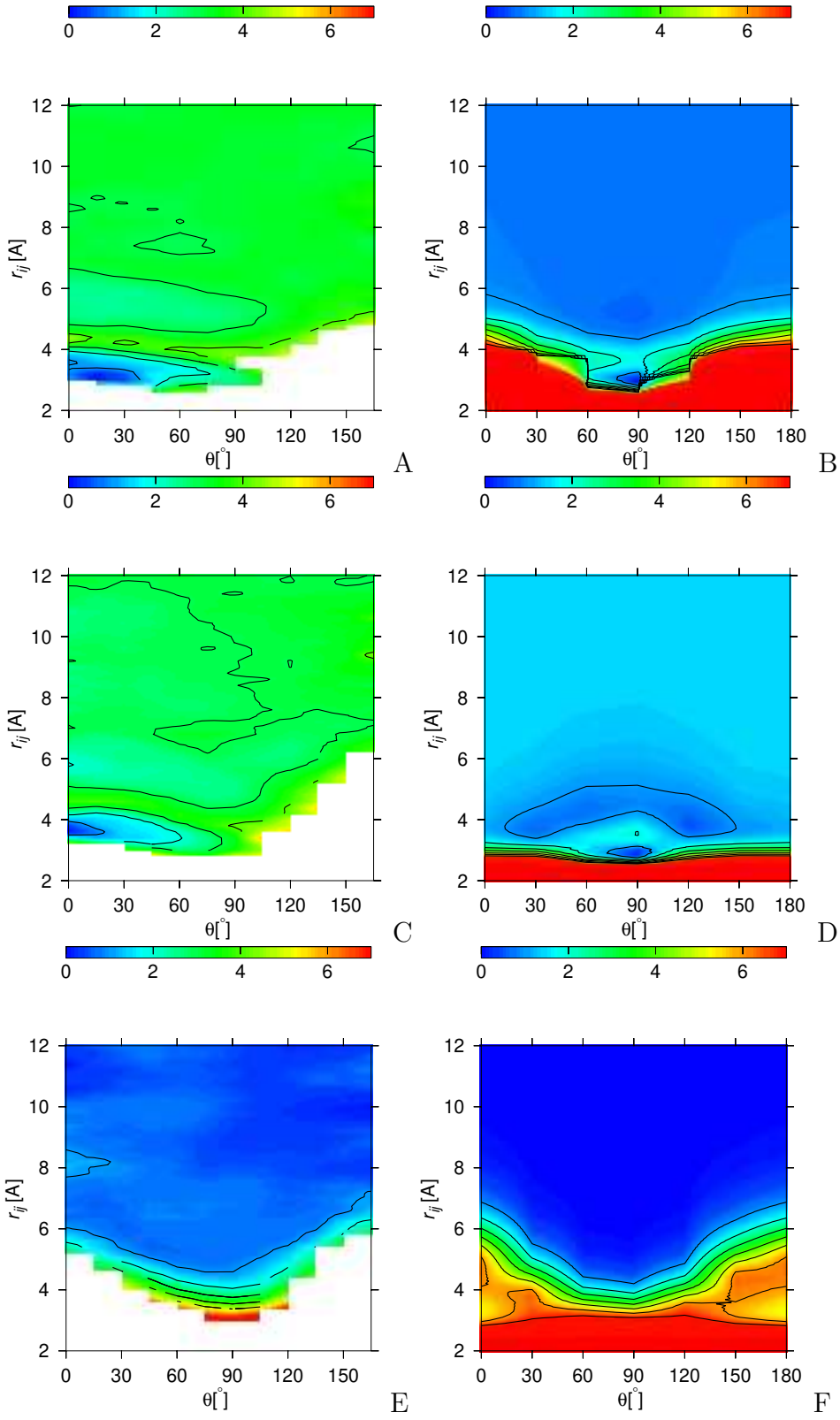


Figure 11: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Na^+ interacting with polar side-chain models: serine (A) and (B), threonine (C) and (D), cysteine (E) and (F), asparagine (G) and (H), glutamine (I) and (J), histidine (K) and (L), tyrosine (M) and (N), and peptide group (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 30 60 90 120 150 180
θ[°]
B
C
D
E
F

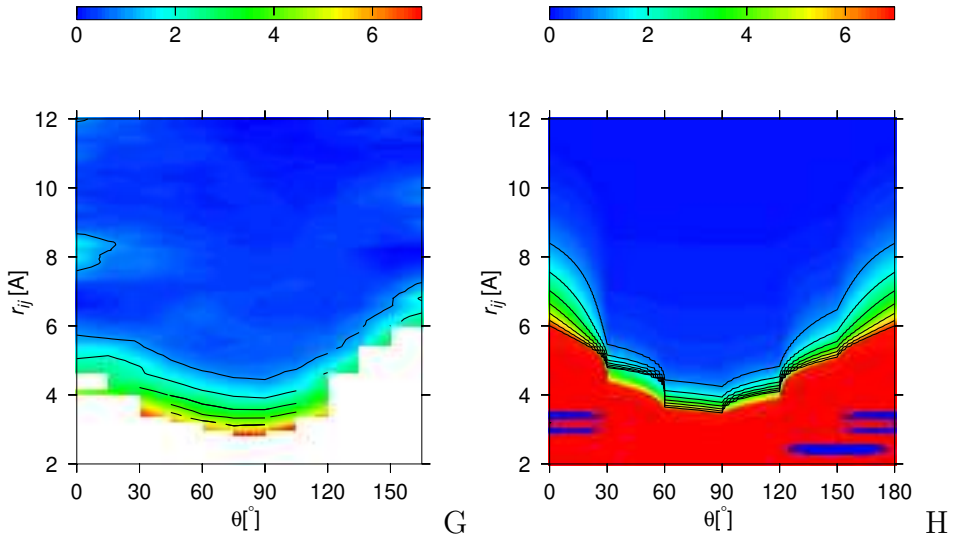
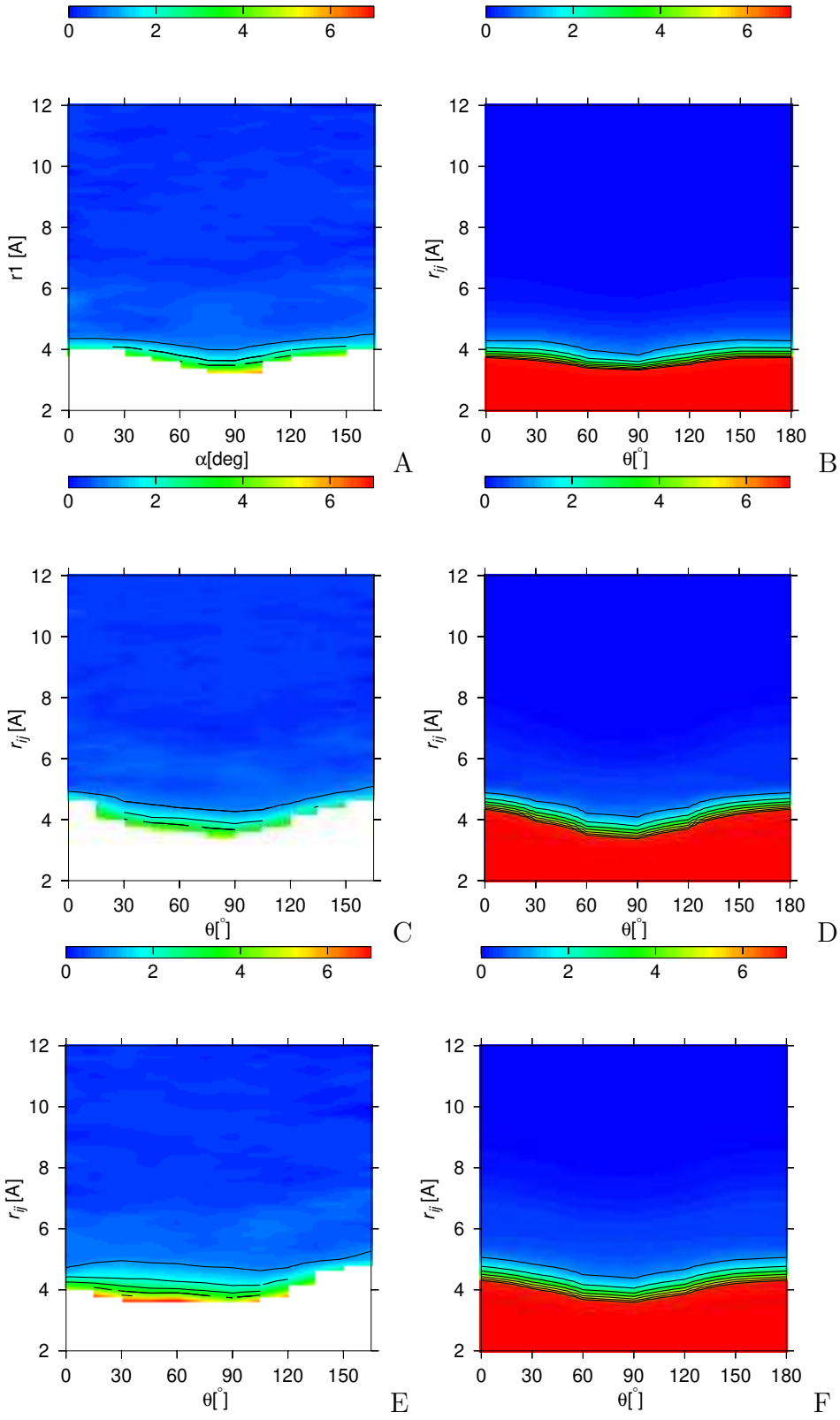
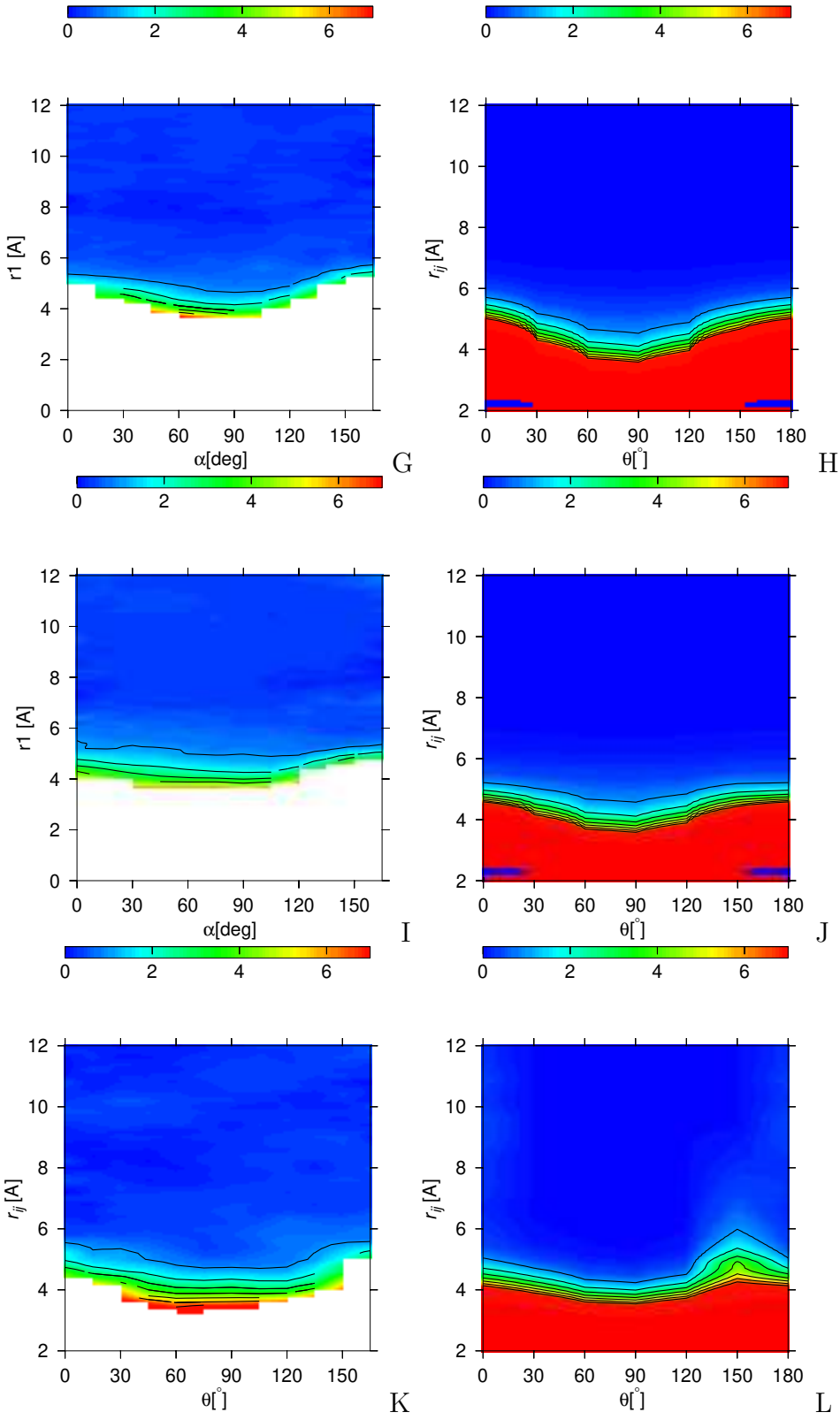


Figure 12: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Na^+ interacting with charged side-chain models: aspartic acid (A) and (B), glutamic acid (C) and (D), lysine (E) and (F), arginine (G) and (H).


0 2 4 6
r1 [A]
α[deg]
A
r_{ij} [A]
θ[°]
B
C
D
E
F


0 2 4 6
r1 [A]
α[deg]
G
r_{ij} [A]
θ[°]
H
I
J
K
L

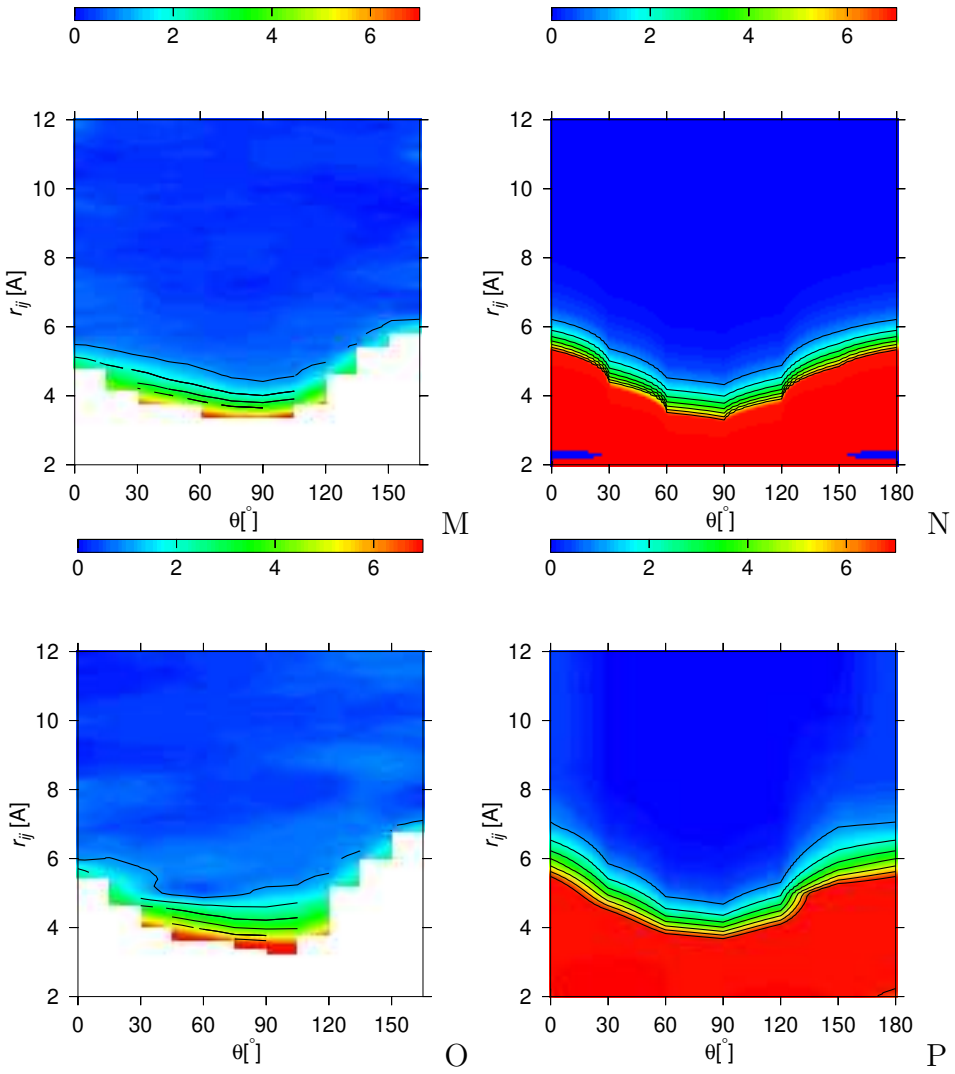
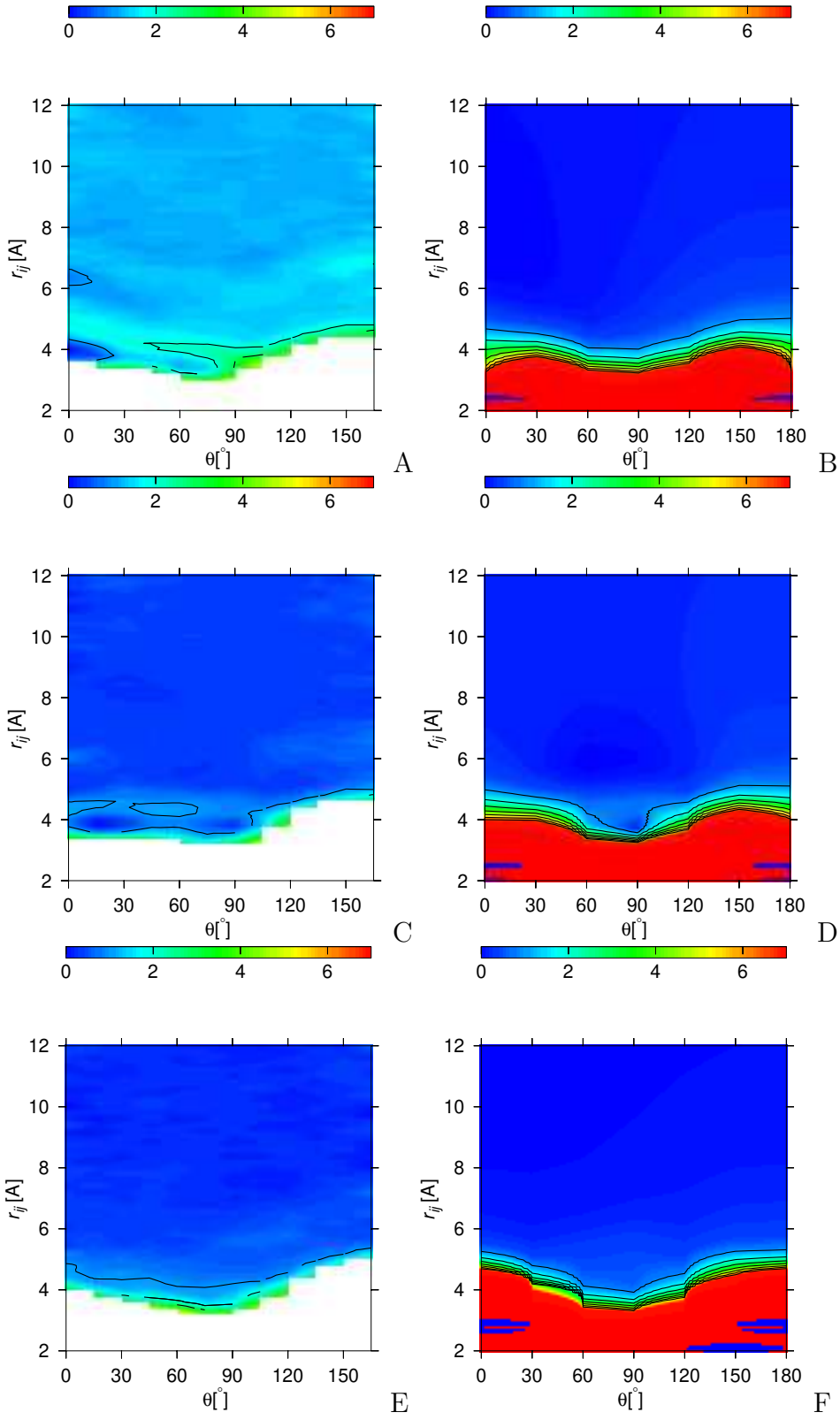
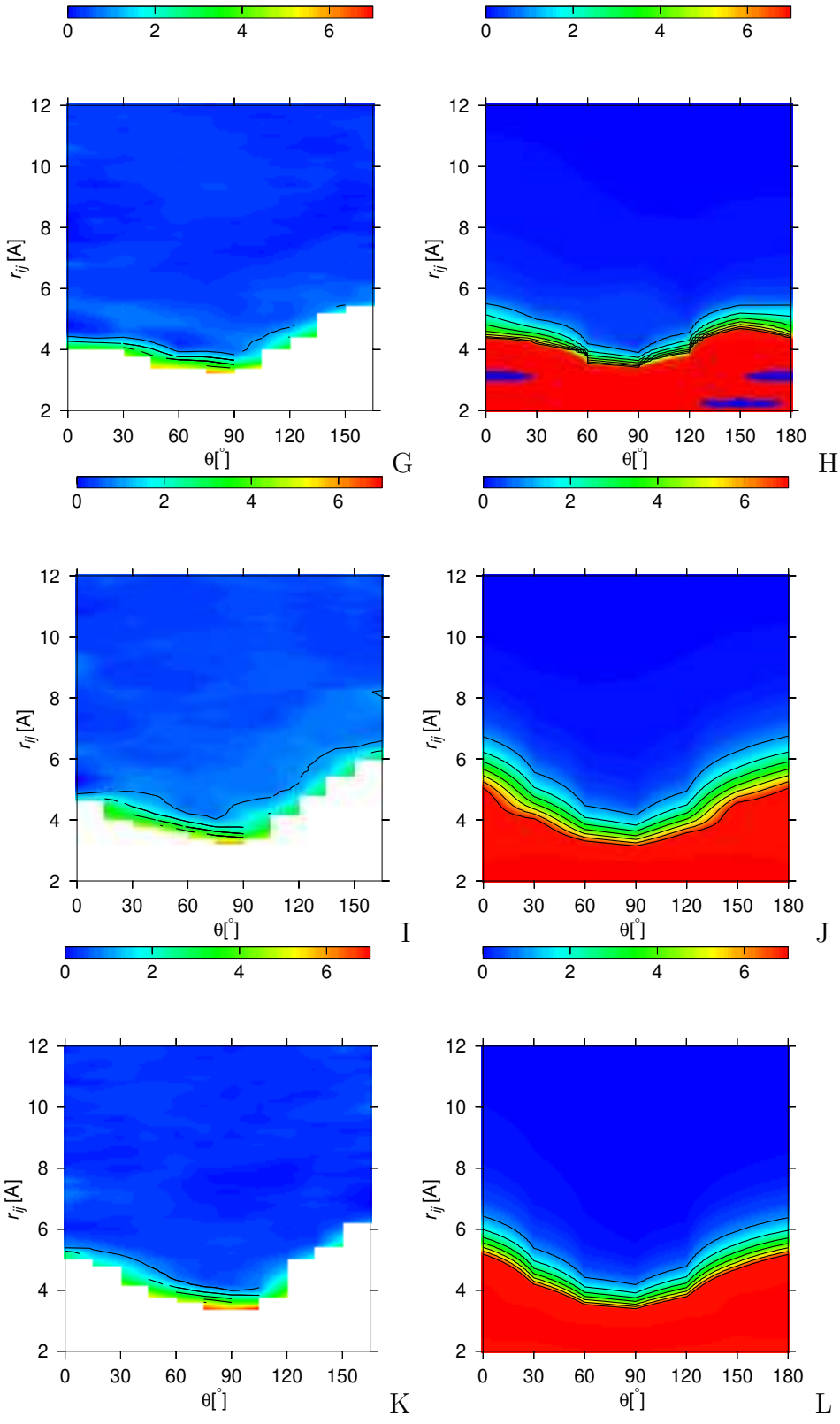


Figure 13: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Cl^- interacting with hydrophobic side-chain models: alanine (A) and (B), proline (C) and (D), valine (E) and (F), leucine (G) and (H), isoleucine (I) and (J), phenylalanine (K) and (L), methionine (M) and (N), tryptophan (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 30 60 90 120 150 180
θ[°]
B
C
D
E
F


0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
G
0 30 60 90 120 150 180
θ[°]
H
0 2 4 6
0 2 4 6
I
J
K
L

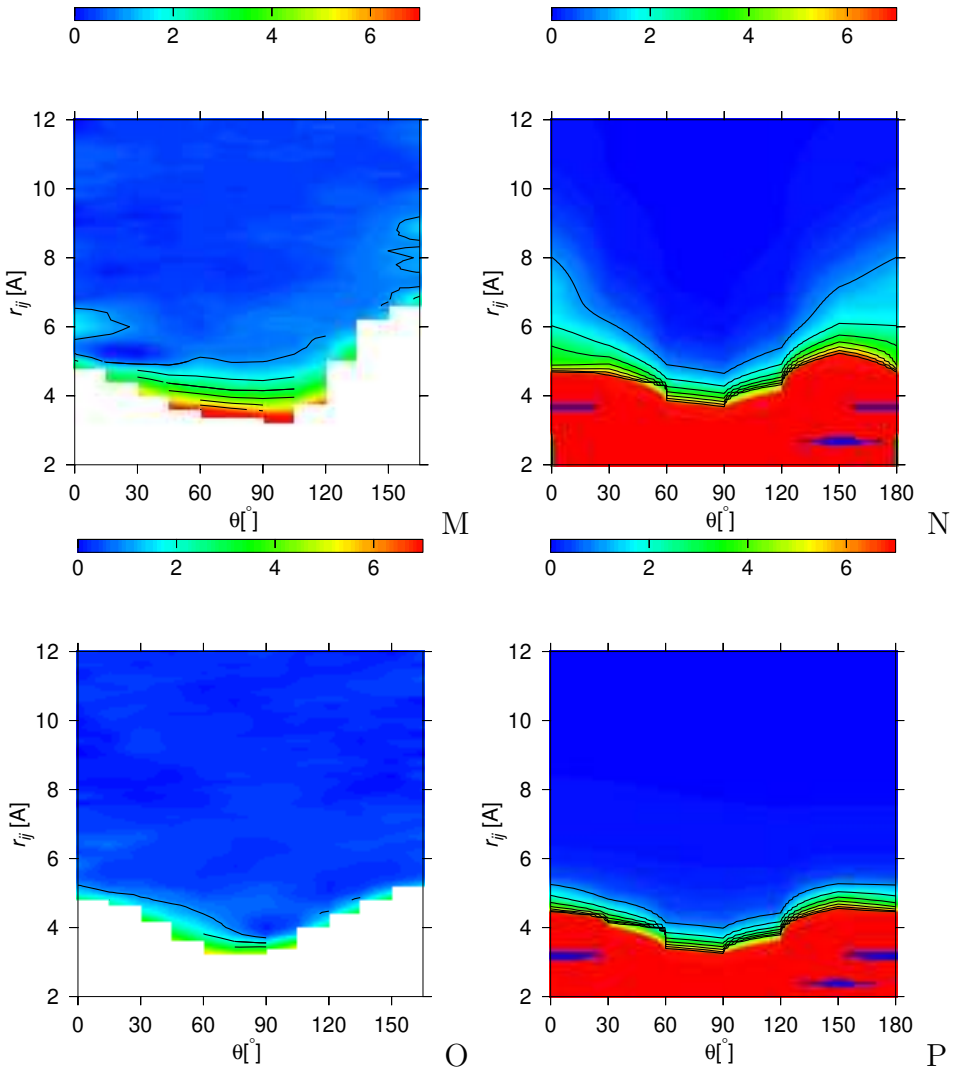
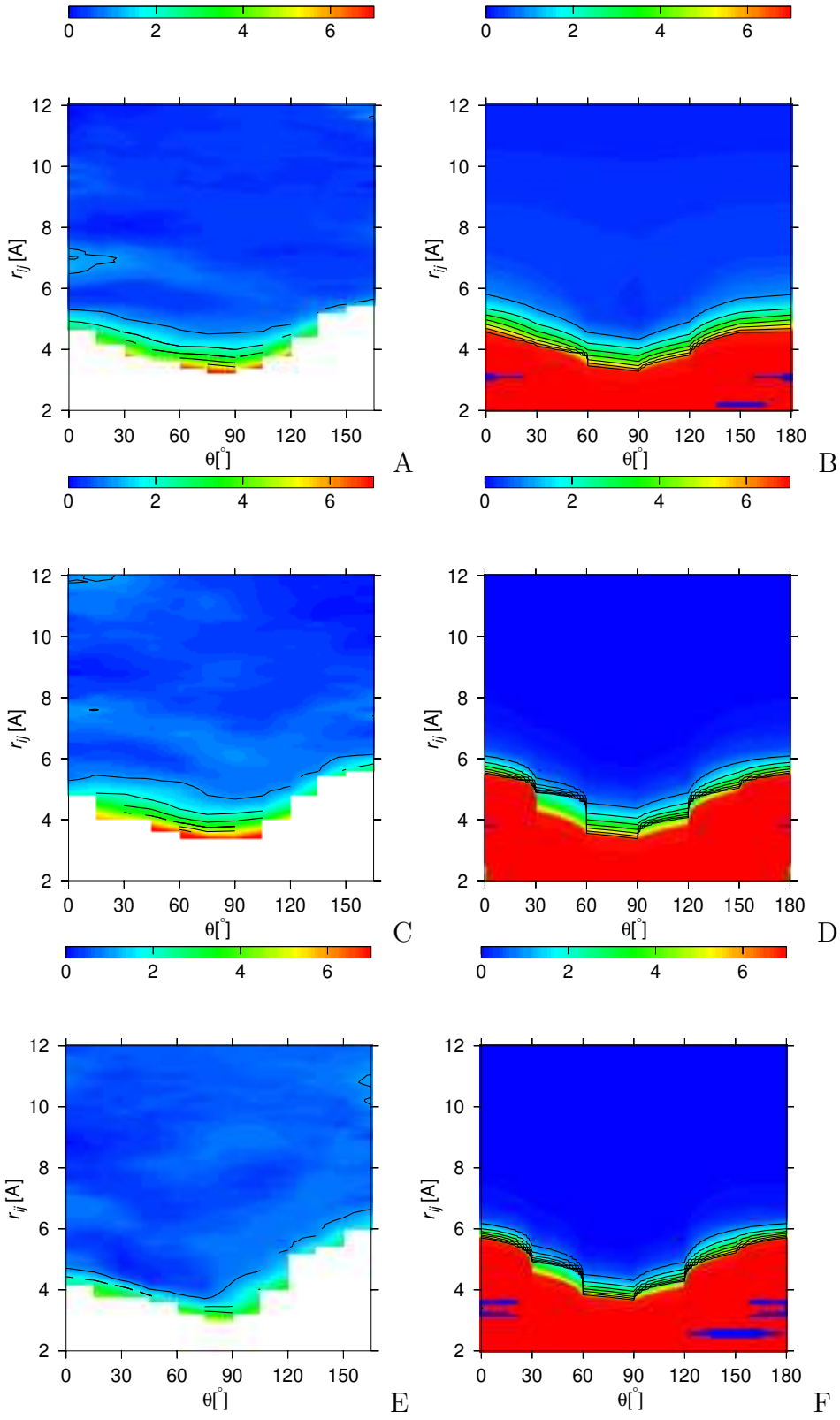


Figure 14: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Cl^- interacting with polar side-chain models: serine (A) and (B), threonine (C) and (D), cysteine (E) and (F), asparagine (G) and (H), glutamine (I) and (J), histidine (K) and (L), tyrosine (M) and (N), and peptide group (O) and (P).


0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
A
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
B
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
C
0 2 4 6
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
D
0 2 4 6
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150
θ[°]
E
12 10 8 6 4 2
r_{ij} [A]
0 30 60 90 120 150 180
θ[°]
F

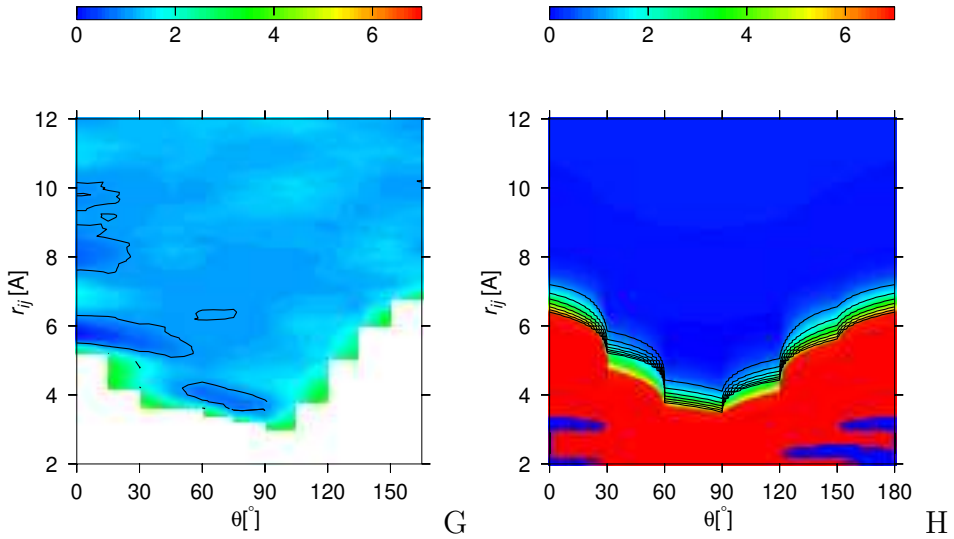


Figure 15: 2D surfaces of the PMF (on the left) and fitted analytical energy function (on the right) for Cl^- interacting with charged side-chain models: aspartic acid (A) and (B), glutamic acid (C) and (D), lysine (E) and (F), arginine (G) and (H).

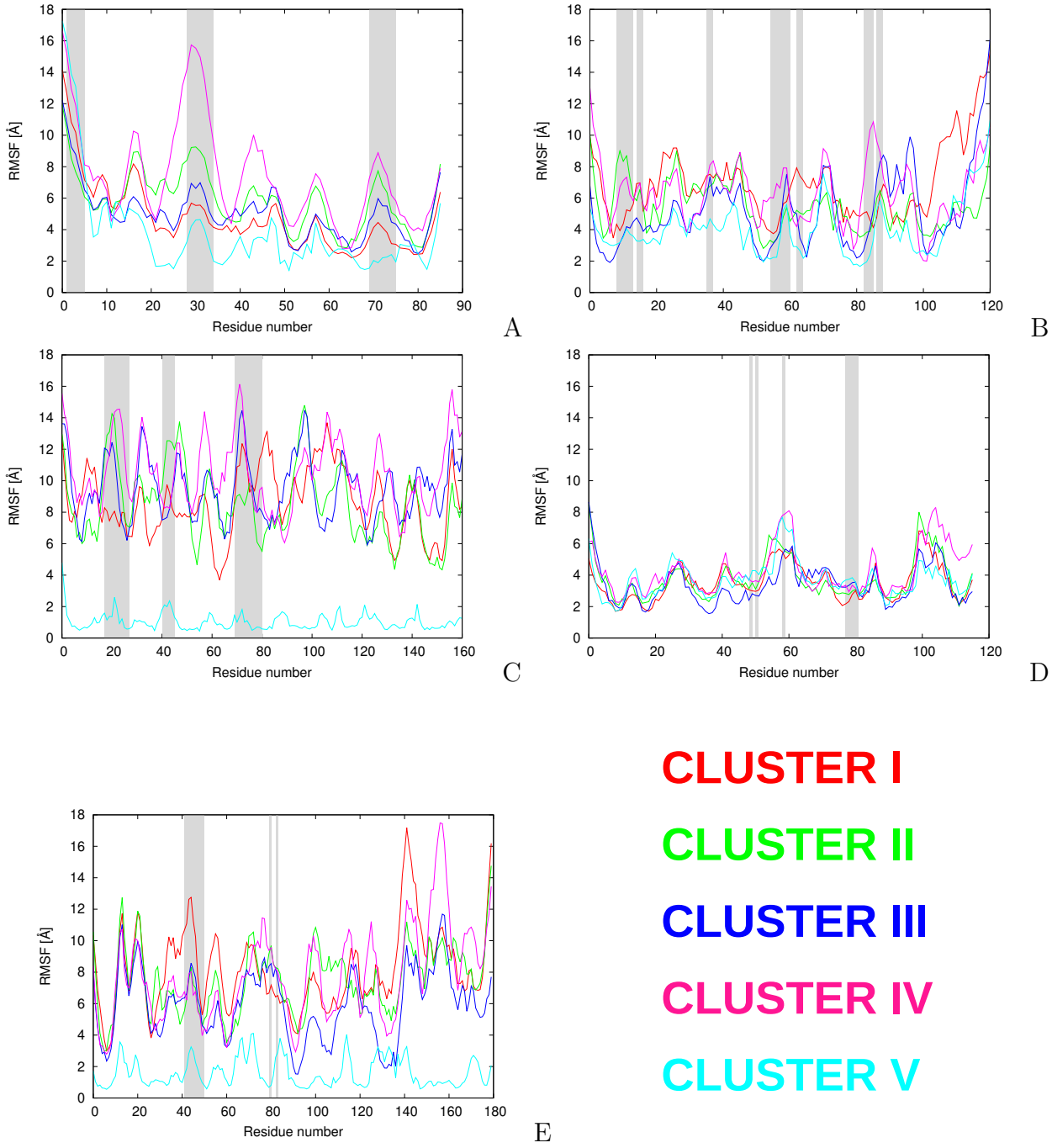
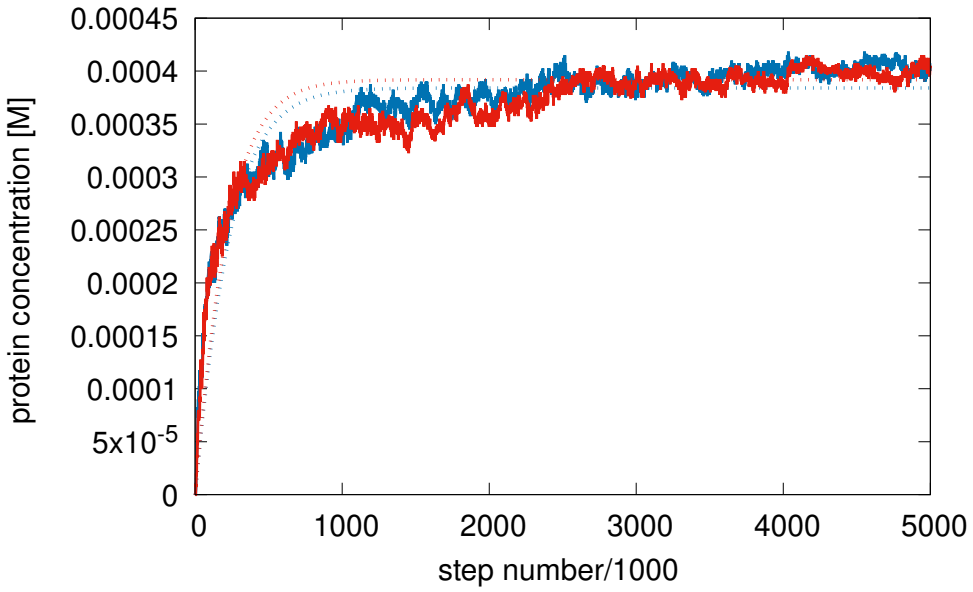
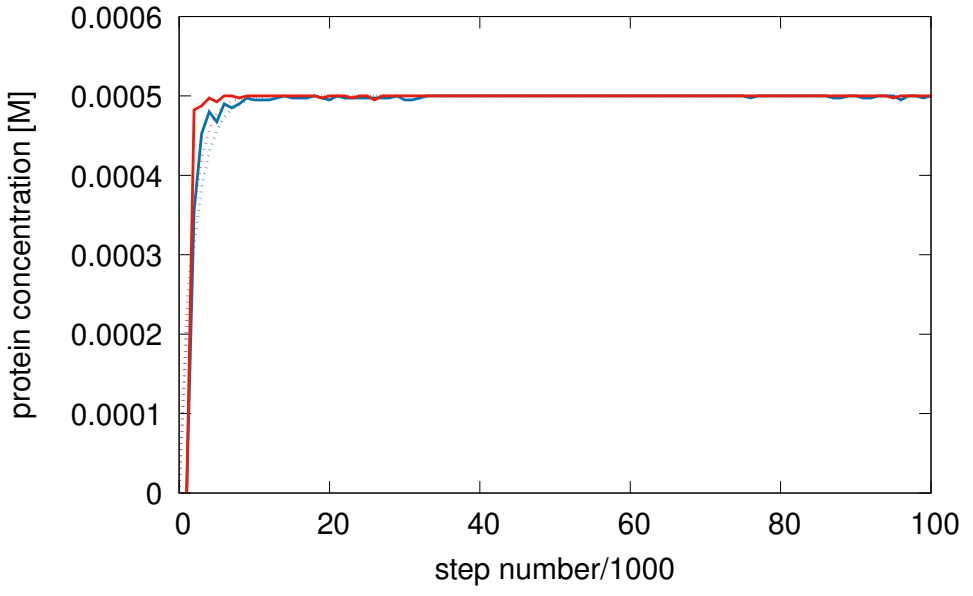


Figure 16: Plots of root-mean-square fluctuations (RMSF) of C^{α} atoms in each cluster for: (A) 4AQO, (B) 6EKG, (C) 4RJ9, (D) 5E56, (E) 2Z2K. Shaded areas indicate the amino acid residues that are in contact with the ion in the native structure. As a reference structure the cluster representative was taken.



A



B

Figure 17: Plots of concentration of unbound structures of 1F6S and metal ions over time with fitted curves for (A) calcium (blue) and magnesium (red) ions and (B) sodium (blue) and potassium (red) ions.