Coarse Point Charge Models For Proteins From Smoothed Molecular Electrostatic Potentials

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Supporting Information

Table SI1. CG charges (in e^-) for the AA residues obtained through the charge fitting algorithm using unsmoothed all-atom Amber99 MEP grids. CG locations were generated at t = 1.25 bohr^2 using the hierarchical merging/clustering algorithm applied to the all-atom Amber MEP function. *g* and *t* stand for *gauche* and *trans*, respectively (see references 54, 55 for details). *rmsdV* and *rmsdμ* are given in kcal/mol and D, respectively. Point numbers refer to Figure 5.

	Conformation	Point 1	Point 2	Point 3	Point 4	Point 5	Point 6	Point 7	Point 8	*rmsdV*	*rmsdμ*
Ala		C	O								
		0.4052	-0.4052							2.00	0.48
Arg		C	O	NH-NH_2	Cζ	NH_2-NH	NH_2-NH_2				
	g-,t,g-,g-									5.16	2.88
	g-,t,g-,t	0.3588	-0.3949	0.2780	0.0555	0.4811	0.2215			4.67	2.86
	g-,t,g+,t									4.54	2.23
	g-,t,t,t									4.84	3.20
Asn		C	O	$H\delta_{tr}$	Oδ	$H\delta_{cis}$					
	t,Nt									2.62	1.01
	t,Og-	0.3990	-0.3940	0.1470	-0.2340	0.0820				2.83	0.95
	t,Og+									2.44	0.87
Asp		C	O	Oδ1	Oδ2						
	t,g+	0.3033	-0.4453	-0.4290	-0.4290					2.85	1.28
Cys		C	O	Sγ	Hγ						
	g-									2.16	0.56
	g+	0.4160	-0.3970	-0.0705	0.0515					3.03	1.55
	t									2.62	1.24
Gln		C	O	Cγ	H_{tr}	Oε	H_{cis}				
	g-,t,Nt									1.90	0.10
	g-,t,Og-	0.3687	-0.4017	0.1768	0.0958	-0.3215	0.0818			1.96	0.20
	g-,t,Og+									1.92	0.39
Glu		C	O	Oε1	Oε2						
	g-,t,g-	0.3296	-0.4476	-0.4410	-0.4410					2.74	0.79
	g-,t,g+									2.91	0.98
Gly		C	O								
		0.3897	-0.3897							1.21	0.28
Hisδ		C	O	Nε	HNδ	HCδ					
	g-,Ng-	0.3902	-0.3982	-0.2306	0.1863	0.0523				2.67	0.86
	t,Ng+									2.93	0.81
Hisε		C	O	HNε	Nδ	HCδ					
	g-,Ng-	0.3538	-0.3898	0.1803	-0.2142	0.0699				2.50	0.66
	t,Ng+									2.71	0.85
Ile		C	O								
	g-,g-									2.02	0.87
	g-,t	0.4042	-0.4042							1.95	0.76
	g+,t									1.96	0.73
Leu		C	O								
	g-,t	0.4116	-0.4116							2.11	0.98
	t,g+									2.09	0.87
Lys		C	O	Nζ							
	g-,g-,t,g-	0.3162	-0.3422	1.0260						5.22	3.78
	g-,g-,t,g+									4.83	3.49

	g-,t,t,g-									4.29	2.90
	g-,t,t,g+									5.15	3.98
Met		C	O	Sδ	CH_3						
	g-,g-,g-									2.38	1.16
	g-,g-,t									2.32	1.18
	g-,t,g-	0.3264	-0.3767	-0.0654	0.1154					2.85	1.54
	g-,t,g+									2.87	1.53
	g-,t,t									2.93	1.61
Phe		C	O	6-ring	Hε1	Hς	Hε2				
	g-,g-	0.3743	-0.3933	-0.0753	0.0425	0.0093	0.0425			2.40	0.27
	t,g+									2.60	0.84
Pro		C	O								
	g+	0.2848	-0.2848							5.40	3.93
Ser		C	O	Oγ	Hγ						
	g-	0.3098	-0.3647	-0.0997	0.1547					3.14	1.18
	g+									4.22	2.08
Thr		C	O	Oγ	Hγ						
	g-	0.3497	-0.4022	-0.1157	0.1682					3.15	1.39
	g+									3.58	1.76
Trp		C	O	5-ring	HCδ1	HNε1	6-ring	HH2	Hς3		
	g-,g-									2.45	0.36
	g-,t									2.35	0.25
	t,g-	0.3731	-0.4027	-0.1380	-0.0963	0.1002	-0.0640	0.0284	0.0068	2.64	0.45
	t,g+									2.31	0.60
	t,t									2.48	0.58
Tyr		C	O	6-ring	Hδ*	Hε*	OH	HH			
	g-,g-	0.3956	-0.4237	-0.0406	0.0498	0.0115	-0.1535	0.1610		2.58	0.54
	t,g+									2.89	0.80
Val		C	O								
	g-	0.4095	-0.4095							2.05	0.69
	t									2.02	0.69

*in the opposite direction of O-H bond.

Table SI2. CG charges (in e^-) for the AA residues obtained through the charge fitting algorithm using unsmoothed Gromos43A1 MEP grids. CG locations were generated at t = 1.3 bohr^2 using the hierarchical merging/clustering algorithm applied to the Gromos43A1 MEP function. *g* and *t* stand for *gauche* and *trans*, respectively (see references 54, 55 for details). *rmsdV* and *rmsdμ* are given in kcal/mol and D, respectively. Point numbers refer to Figure 6.

	Conformation	Point 1	Point 2	Point 3	Point 4	Point 5	Point 6	Point 7	Point 8	*rmsdV*	*rmsdμ*
Ala		H	O								
		0.2050	-0.2050							1.30	0.46
Arg		H	O	Cζ							
	g-,t,g-,g-									3.18	0.73
	g-,t,g-,t	0.2068	-0.2068	1.0000						3.56	0.74
	g-,t,g+,t									3.49	0.44
	g-,t,t,t									3.53	0.98
Asn		H	O	Oδ	$H\delta_{tr}$	$H\delta_{cis}$					
	t,Nt									1.50	0.61
	t,Og-	0.1952	-0.1952	-0.1943	0.1104	0.0840				1.53	0.70
	t,Og+									1.39	0.46
Asp		H	O	Oδ1	Oδ2						
	t,g+	0.1868	-0.1868	-0.5000	-0.5000					2.15	0.60
Cys		H	O	Sγ							
	g-									0.95	0.50
	g+	0.2051	-0.2051	-0.0299	0.0299					0.94	0.44
	t									0.93	0.43
Gln		H	O	H_{cis}	Oε	H_{tr}					
	g-,t,Nt									1.32	0.28
	g-,t,Og-	0.2086	-0.2086	0.0850	-0.2031	0.1182				1.20	0.30
	g-,t,Og+									1.29	0.58
Glu		H	O	Oε1	Oε2						
	g-,t,g-	0.2029	-0.2029	-0.5000	-0.5000					1.95	0.51
	g-,t,g+									2.01	0.59
Gly		H	O								
		0.2050	-0.2050							0.55	0.11
Hisδ		H	O	HNδ	Nε						
	g-,Ng-	0.1972	-0.1972	0.2623	-0.2623					1.22	0.50
	t,Ng+									1.25	0.46
Hisε		H	O	HNε	Nδ						
	g-,Ng-	0.1941	-0.1941	0.2729	-0.2729					1.11	0.40
	t,Ng+									1.16	0.51
Ile		H	O								
	g-,g-									0.90	0.46
	g-,t	0.2052	-0.2052							0.89	0.46
	g+,t									0.89	0.46
Leu		H	O								
	g-,t	0.2052	-0.2052							0.88	0.46
	t,g+									0.90	0.46
Lys		H	O	Nζ							
	g-,g-,t,g-									1.10	1.06
	g-,g-,t,g+	0.2051	-0.2051	1.0000						1.06	0.65
	g-,t,t,g-									1.03	0.52
	g-,t,t,g+									1.08	0.67
Met		H	O								
	g-,g-,g-	0.2051	-0.2051							0.87	0.46
	g-,g-,t									0.87	0.46
	g-,t,g-									0.85	0.46

	g-,t-,g+									0.85	0.46
	g-,t,t									0.86	0.46
Phe		H	O	6-ring	Hε1	Hς	Hε2				
	g-,g-	0.2021	-0.2021	-0.0936	0.0386	0.0163	0.0386			1.17	0.26
	t,g+									1.40	0.59
Pro		H	O								
	g+	0.2050	-0.2050							0.92	0.46
Ser		H	O	Oγ	Hγ						
	g-	0.2004	-0.2004	-0.1466	0.1466					1.15	0.22
	g+									1.38	0.53
Thr		H	O	Oγ	Hγ						
	g-	0.2071	-0.2071	-0.1459	0.1459					1.20	0.36
	g+									1.26	0.47
Trp		H	O	5-ring	HNε1	6-ring	HH2	Hς3	Hε3		
	g-,g-									1.13	0.58
	g-,t									1.16	0.56
	t,g-	0.2051	-0.2051	-0.1232	0.1553	-0.1409	0.0466	0.0319	0.0303	1.23	0.57
	t,g+									0.98	0.91
	t,t									1.07	0.45
Tyr		H	O	6-ring	HH	OH	Hε	Hδ			
	g-,g-	0.2188	-0.2188	0.04148	0.1523	-0.1988	0.0153	0.0165		1.31	0.26
	t,g+									1.62	0.64
Val		H	O								
	g-	0.2052	-0.2052							0.93	0.46
	t									0.93	0.46

*in the opposite direction of O-H bond.

Table SI6. Electrostatic properties of the Gromos43A1-based CG model of small peptides *vs*. their corresponding all-atom version. *rmsdV* and *rmsdμ* are given in kcal/mol and D, respectively. Electric charges are given in e^-. (a) no charge fitting applied, (b) charge fitting applied to end charges q_{end} only, (c) charge fitting applied to all CG charges, (d) charge fitting applied to Basdevant's model.

2EVQ	197 atoms			
q	1.0			
μ (all-atom) [a]	3.20, -0.04, -69.06			
	(a)	(b)	(c)	(d)
No. of CGs	51	51	51	28
rmsdV	1.94	1.86	1.09	5.60
rmsdμ	0.44	0.88	0.04	1.44
μ [a]	2.93, -0.31, -69.28	2.78, 0.08, -69.83	3.19, -0.03, -69.03	3.45, -0.94, -67.95
q_{end}	±1.0000	±1.0222		
1BXX	110 atoms			
q	0.0			
μ (all-atom) [a]	17.25, 0.86, -11.91			
	(a)	(b)	(c)	(d)
No. of CGs	28	28	28	15
rmsdV	3.09	2.99	2.28	6.82
rmsdμ	3.28	2.05	0.98	1.94
μ [a]	14.21, 0.48, -13.10	15.76, 1.90, -12.86	17.45, 1.81, -12.00	19.12, 0.34, -12.03
q_{end}	±1.0000	±1.0254		
1BC5	90 atoms			
q	-1.0			
μ (all-atom) [a]	-314.89, -289.54, 5.97			
	(a)	(b)	(c)	(d)
No. of CGs	29	29	29	13
rmsdV	2.46	2.20	1.60	7.61
rmsdμ	0.08	1.91	2.53	3.18
μ [a]	-314.87, -289.47, 5.94	-314.17, -291.31, 5.97	-313.82, -291.35, 4.57	-314.01, -287.40, 3.79
q_{end}	±1.0000	±1.0272		
2RD4	88 atoms			
q	0.0			
μ (all-atom) [a]	40.10, 25.05, -46.97			
	(a)	(b)	(c)	(d)
No. of CGs	20	20	20	12
rmsdV	3.37	2.70	1.52	7.72
rmsdμ	4.87	2.54	0.47	3.23
μ [a]	37.07, 21.56, -45.44	39.62, 22.94, -48.28	39.68, 24.86, -47.08	40.01, 24.96, -43.75
q_{end}	±1.0000	±1.0579		

[a] x, y, and z components of μ.

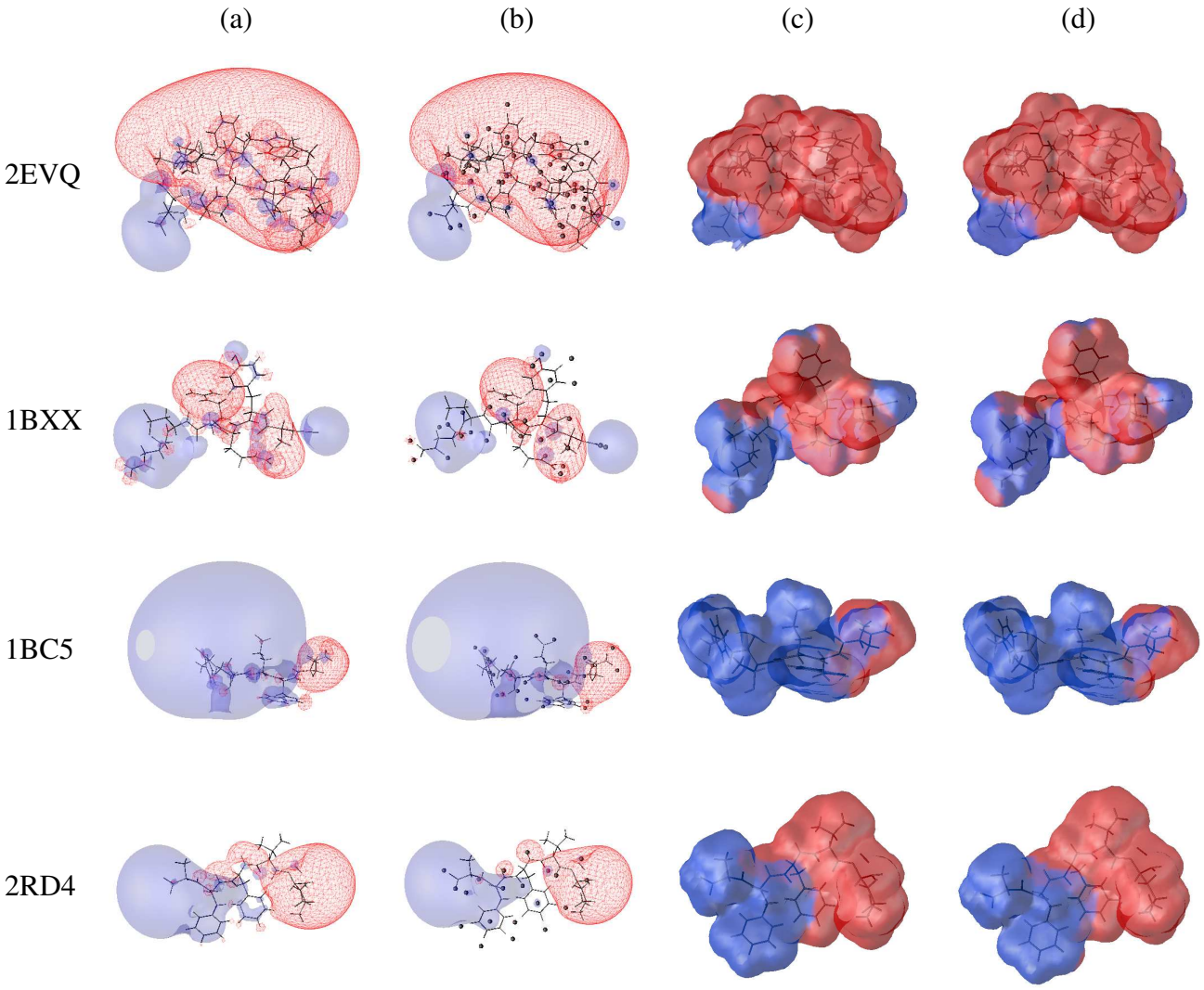

Figure SI7. Gromos43A1 MEP isocontours (blue plain surface: -0.07, red mesh: 0.07 e^-/bohr) and MEP projected on the ED surface defined at 0.0002 e^-/bohr^3 (blue: negative, red: positive) of peptides 2EVQ, 1BXX, 1BC5, and 2RD4. (a) unsmoothed all-atom MEP, (b) CG with fitted q_{end} MEP with CGs (black spheres), (c) all-atom MEP on ED isocontour, and (d) CG with fitted q_{end} MEP on ED isocontour.

3D structure and charges of the all-atom and coarse point charge models generated for the four peptides (PDB codes 2EVQ, 1BXX, 1BC5, and 2RD4) and structure KcsA (PDB code 1BL8) can be downloaded from http://perso.fundp.ac.be/~lleherte/JCTC_SI/.