

Table 1 Torsion Angles along the Lateral Chains of the Arginine Molecules
 Residue torsion angles

Residue	CHI1	CHI2	CHI3	CHI4	CHI5	CHI6
CH1	N- CA-CB- CG					
CH2	CA-CB- CG- CD					
CH3	CB- CG- CD- NE					
CH4	CG- CD- NE- CZ					
CH5	CD- NE- CZ- NH1					
CH6	CD- NE- CZ- NH2					
Arg 1	-69.33	169.85	179.39	81.30	-177.75	1.83
Arg 2	68.52	173.67	-59.95	-81.52	-178.02	3.55
Arg 3	-71.29	-177.32	49.58	70.79	-179.19	0.04
Arg 4	35.30	-179.81	-39.88	106.73	176.75	-5.62
Arg 5	60.31	159.25	172.29	96.84	-4.89	178.28
Arg 6 D1	-174.05	-168.66	172.77	-77.25	-179.29	-1.26
Arg 6 D2	173.99	-32.86	61.14	145.54	-2.87	-179.52

Table 2 Sulphonate –Water Hydrogen Bond Distances

Residue	SO ⁻ - H ₂ O
Calix 1	2.86; 2.89; 2.96; 2.84 3.06 2.75; 2.99 2.90; 2.76; 2.96
Calix 2	2.65; 2.95-2.97; 2.70-3.04 2.72; 2.94; 2.81 2.74; 3.17 2.58-2.79
Calix 3	2.66 2.76 2.75-2.40 2.72 2.33-2.64 2.94-2.74 2.86 2.75
Calix 4	2.54 3.04 2.81-2.83 2.68 2.44-2.59

Table 3 Hydrogen Bond Distances For the Arginine Molecules

Residue	NH ₃ ⁺ -H ₂ O	COO ⁻ -H ₂ O	NH ₂ ⁺ -H ₂ O	NH ₂ -H ₂ O	NH-H ₂ O	NH ₃ ⁺ -SO ⁻	COO ⁻ - SO ⁻	NH ₂ ⁺ -SO ⁻	NH ₂ - SO ⁻	NH- SO ⁻
Arg 1	3.03	2.60; 2.70	-	3.05	-	2.85	-	3.03; 2.94	3.02	2.95
Arg 2	-	3.03	3.20-3.21	-	3.01	2.84-2.88	2.73	2.80-2.96	2.96-3.03	3.26
Arg 3	2.56	3.12	-	-	-	2.75	2.62	2.99	3.01	2.90
Arg 4	3.01	2.60	-	2.92	-	2.81-2.61	3.41-3.42	2.93	2.92-2.88	3.09
Arg 5	2.7	2.63; 3.31	3.02	-	3.14	2.86	3.05	2.91	2.88-2.72	-