

Table 3. Description of the geometries of heparin fragments in the bound state

	IL-8		SDF-1		RANTES		CDF		PF-4*	
	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ
α -D-Glc(1-4)	76	-147 [†]	57	-166 [†]	77	-149 [†]	92	-140 [†]	76	-147 [†]
β -L-IdoA(1-4)	-70 [†]	-111	-68 [†]	-103	-74 [†]	-112	-75 [†]	-125	-71 [†]	-107
α -D-Glc(1-4)	78	-150 [†]	82	-155 [†]	76	-139 [†]	81	-148 [†]	75	-149 [†]
β -L-IdoA(1-4)	-76 [†]	-103	-39 [†]	-85	-80 [†]	-125	-75 [†]	-105	-72 [†]	-99
α -D-Glc(1-4)	144	-91 [‡]	80	-156 [†]	92	-60 [‡]	134	-92 [‡]	123	-88 [‡]
β -L-IdoA(1-4)	-84 [‡]	176	-137 [†]	-122	-90 [‡]	-159	-83 [‡]	178	-80 [‡]	-178
α -D-Glc(1-4)	81	-153 [†]	99	-101 [†]	83	-109 [†]	79	-148 [†]	82	-145 [†]
β -L-IdoA(1-4)	-74 [†]	-102	-75 [†]	-107	-78 [†]	-173	-69 [†]	-105	-67 [†]	-114
α -D-Glc(1-4)	78	-150 [†]	75	-154 [†]	124	-97 [‡]	74	-149 [†]	73	-151 [†]
β -L-IdoA(1-4)	-70 [†]	-103	-58 [†]	-94	-61 [†]	-146	-69 [†]	-106	-71 [†]	-107
α -D-Glc(1-4)	62	-153 [†]	68	-173 [†]	101	-79 [‡]	71	-148 [†]	74	-151 [†]
β -L-IdoA(1-4)	-60 [†]	-95	-64 [†]	-97	-81 [†]	-176	-68 [†]	-102	-82 [†]	-106
α -D-Glc(1-4)	117	-77 [‡]	49	-174 [†]	49	180 [†]	136	-90 [‡]	115	-85 [‡]
β -L-IdoA(1-4)	-75 [‡]	177	-64 [†]	-97			-78 [‡]	174	-79 [‡]	-177
α -D-Glc(1-4)	72	-160 [†]					72	-166 [†]	79	-149 [†]
β -L-IdoA(1-4)	-68 [†]	-103					-71 [†]	-103	-77 [†]	-106
α -D-Glc(1-4)	88	-154 [†]					80	-146 [†]	120	-85 [‡]
β -L-IdoA(1-4)									-79	-179
α -D-Glc(1-4)									79	-148 [†]
β -L-IdoA(1-4)									-67 [†]	-104

*Values averaged from the two heparin fragment (deviation less than 1° after optimization).

[†]With adjacent L-IdoA ring in ¹C₄ conformation.

[‡]With adjacent L-IdoA ring in ²S_O conformation.