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Table S1: ^1H NMR Chemical Shifts (ppm) of Ca^{2+} -Free FVII EGF1 at 25° C, pH 5.56^a

residue	NH	C^αH	C^βH	C^γH	C^δH	other
S45		4.16	3.99, 3.99			
D46	8.82	4.62	2.61, 2.72			
G47	8.46	3.98, 3.98				
D48	8.10	4.70	2.73			
Q49	8.84	4.20	1.99 ($\text{H}^\beta 2$) 2.28 ($\text{H}^\beta 3$)	2.39		6.76 ($\text{H}^\varepsilon 21$), 7.60 ($\text{H}^\varepsilon 22$)
C50	9.27	4.20	2.96, 3.05			
A51	8.03	4.13	1.45			
S52	7.64	4.40	3.81, 3.89			
S53	7.96	4.12	3.90, 3.90			
P54		4.14	1.48 ($\text{H}^\beta 2$) 1.59 ($\text{H}^\beta 3$)	0.42, 1.33	3.33, 3.36	
C55	7.74	4.40	2.26 ($\text{H}^\beta 3$) 2.62 ($\text{H}^\beta 2$)			
Q56	8.51	4.20	1.70 ($\text{H}^\beta 2$) 2.06 ($\text{H}^\beta 3$)	2.40		6.81 ($\text{H}^\varepsilon 21$), 7.34 ($\text{H}^\varepsilon 22$)
N57	9.08	3.95	1.03, 1.78			7.21 ($\text{H}^\delta 21$), 8.08 ($\text{H}^\delta 22$)
G58	8.78	3.64, 4.00				
G59	7.32	3.40 ($\text{H}^\alpha 3$) 4.26 ($\text{H}^\alpha 2$)				
S60	8.52	4.77	3.96			
C61	8.90	5.34	2.90, 3.06			
K62	9.40	4.78	1.83, 1.91	1.53	1.75, 1.75	2.95 ($\text{C}^\epsilon\text{H}_2$)
D63	8.82	4.76	2.58, 2.76			
Q64	8.27	4.54	1.76, 1.97	2.13		6.87 ($\text{H}^\varepsilon 21$), 7.32 ($\text{H}^\varepsilon 22$)
L65	9.06	3.96	1.57, 1.92	1.57	0.89, 0.94	
Q66	8.40	4.40	2.04	2.33, 2.74		6.82, 7.56 ($\text{C}^\epsilon\text{H}_2$)
S67	8.00	4.68	3.72, 3.79			5.80 (O^γH)
Y68	8.39	5.47	2.77 ($\text{H}^\beta 3$) 3.01 ($\text{H}^\beta 2$)			6.79 (C^δH , $\text{C}^\epsilon\text{H}$)
I69 -	9.14	4.27	1.53	0.83, 1.29		0.59 ($\text{C}^\gamma\text{H}_3$), 0.75 ($\text{C}^\delta\text{H}_3$)
C70	8.76	5.52	2.75 ($\text{H}^\beta 3$) 2.90 ($\text{H}^\beta 2$)			
F71	9.50	4.74	3.01 ($\text{H}^\beta 2$) 3.15 ($\text{H}^\beta 3$)			7.25 (C^δH , $\text{C}^\epsilon\text{H}$, C^ζH)
C72	8.89	4.77	2.71 ($\text{H}^\beta 2$) 3.33 ($\text{H}^\beta 3$)			
L73	8.51	4.64	1.72, 2.05	1.72		1.02 ($\text{C}^\delta 2\text{H}_3$), 1.08 ($\text{C}^\delta 1\text{H}_3$)
P74		4.33	1.87 ($\text{H}^\beta 2$) 2.38 ($\text{H}^\beta 3$)	2.07, 2.12	3.78, 3.89	
A75	7.55	4.03	0.84			
F76	8.04	5.24	2.74 ($\text{H}^\beta 2$) 3.06 ($\text{H}^\beta 3$)			6.88 (C^δH), 7.18 ($\text{C}^\epsilon\text{H}$), 7.23 (C^ζH)
E77	9.24	4.82	1.96, 2.02	1.96		
G78	8.01	3.76, 4.91				
R79	9.26	3.91	1.77, 1.97	1.63	3.12, 3.15	7.02 ($\text{N}^\epsilon\text{H}$)
N80	9.11	5.66	2.43, 3.54			6.84 ($\text{H}^\delta 21$), 7.46 ($\text{H}^\delta 22$)
C81	7.86	4.06	3.09, 3.52			
E82	10.38	3.96	1.89 ($\text{H}^\beta 3$) 2.16 ($\text{H}^\beta 2$)	2.42, 2.55		
T83	8.70	4.61	3.81	1.17		
H84	9.21	4.41	3.15			8.51 ($\text{H}2$), 7.11 ($\text{H}4$)
K85	8.47	3.86	1.31 ($\text{H}^\beta 2$) 1.70 ($\text{H}^\beta 3$)	1.00, 1.17	1.56	2.83 ($\text{C}^\epsilon\text{H}_2$)

^aChemical shifts are referenced to the H_2O signal at 4.766 ppm and are accurate to ± 0.02 ppm. Where degeneracy of shifts is confirmed from DQ experiments, the shifts are written separately, whereas cases where degeneracy is assumed only one number is written. Stereospecifically assigned resonances are indicated.

Table S2: Hydrogen bonds that were observed in more than 6 of the 23 final structures.

donor	acceptor	number ^a	distance (Å) ^b	angle (°) ^c
Ala ⁵¹ HN	Gln ⁴⁹ O	8	2.10±0.03	138±1
Ser ⁵³ HN	Cys ⁵⁰ O	8	2.41±0.23	155±14
Gln ⁵⁶ HN	Asn ⁸⁰ O	8	2.20±0.12	165±10
Gly ⁵⁹ HN	Gln ⁵⁶ O	7	2.09±0.01	136±1
Ser ⁶⁰ HN	Phe ⁷¹ O	19	2.35±0.20	160±10
Lys ⁶² HN	Ile ⁶⁹ O	7*	2.15±0.08	139±3
Gln ⁶⁴ HN	Ser ⁶⁷ O	17*	2.08±0.02	146±4
Ile ⁶⁹ HN	Lys ⁶² O	7*	2.28±0.08	141±10
Cys ⁷⁰ HN	Arg ⁷⁹ O	12	2.60±0.19	144±6
Phe ⁷¹ HN	Ser ⁶⁰ O	13*	2.12±0.08	149±8
Phe ⁷⁶ HN	Leu ⁷³ O	13*	2.16±0.07	146±9
Cys ⁸¹ HN	Gly ⁷⁸ O	21*	2.22±0.10	134±11
Lys ⁸⁵ HN	Ala ⁷⁵ O	12	2.13±0.04	141±3

^aThe number of structures of the final 23 for which a hydrogen bond is observed. Hydrogen bonds are counted if the hydrogen-acceptor distance is less than 2.9 Å and the donor-hydrogen-acceptor angle is greater than 135°. Asterisks (*) indicate hydrogen bonds for which a distance restraint was applied in the final structure calculations. ^bThe mean hydrogen-acceptor distance (±SD) in the structures for which a hydrogen bond has been observed. ^cThe angle is the mean donor-hydrogen-acceptor angle (±SD) in the structures for which a hydrogen bond has been observed.

Figure S1: Region of a TOCSY spectrum. A squared sinebell shifted 75° was applied in both dimensions, over 130 ms in t_2 (direct dimension) and over 34 ms in t_1 (indirect dimension). The solvent resonance has been removed by deconvolution of the FID with a sinebell convolution function defined over 20 points. A linear baseline correction was applied.

Figure S2: Comparison of H^N and H^α secondary chemical shifts of the N-terminal EGF-like domains from factors VII, IX and X (63,64). The secondary chemical shifts were based on 'random coil' chemical shifts determined by Merutka *et al.* (62). The chemical shifts of FVII EGF1 are reported in Table S1, supporting information.



