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SUPPORTING INFORMATION

Table S1: ^1H chemical shifts of C1r-EGF

residue	H^{N}	$\text{C}^{\alpha}_{\text{H}}$	$\text{C}^{\beta}_{\text{H}}$	others
Ala123	-	4.13	$\text{C}^{\beta}_{\text{H}_3}$ 1.52	
Val124	8.50	4.13	2.06	$\text{C}^{\gamma}_{\text{H}_3}$ 0.91
Asp125	8.50	4.57	2.53, 2.67	
Leu126	8.28	4.28	1.57	$\text{C}^{\gamma}_{\text{H}}$ 1.57, $\text{C}^{\delta}_{\text{H}_3}$ 0.83, 0.88
Asp127	8.47	4.63	2.48, 2.85	
Glu128	8.44	4.09	2.00, 2.10	$\text{C}^{\gamma}_{\text{H}_2}$ 2.26, 2.32
Cys129	9.02	4.01	2.9	
Ala130	8.07	4.13	$\text{C}^{\beta}_{\text{H}_3}$ 1.32	
Ser131	8.20	4.21	3.82, 3.87	
Arg132	8.18	4.29	1.68, 1.78	$\text{C}^{\gamma}_{\text{H}_2}$ 1.48, 1.55, $\text{C}^{\delta}_{\text{H}_2}$ 2.94, $\text{N}^{\delta}_{\text{H}}$ 7.07
Ser133	7.97	4.38	3.86	
Lys134	8.05	4.38	1.74, 1.87	$\text{C}^{\gamma}_{\text{H}_2}$ 1.44, $\text{C}^{\delta}_{\text{H}_2}$ 1.63, $\text{C}^{\epsilon}_{\text{H}_2}$ 2.95
Ser135	8.27	4.4	3.85, 3.91	
Gly136	8.46	3.99		
Glu137	8.38	4.22	1.90, 2.05	$\text{C}^{\gamma}_{\text{H}_2}$ 2.23
Glu138	8.47	4.22	1.92, 2.04	$\text{C}^{\gamma}_{\text{H}_2}$ 2.23
Asp139	8.10	4.81	2.45, 2.70	
Pro140	-	4.36	1.92, 2.20	$\text{C}^{\gamma}_{\text{H}_2}$ 1.98, $\text{C}^{\delta}_{\text{H}_2}$ 3.74
Gln141	8.46	4.52	1.82, 2.02	$\text{C}^{\gamma}_{\text{H}_2}$ 2.35, $\text{N}^{\gamma}_{\text{H}_2}$ 6.83, 7.57
Pro142	-	4.19	1.16, 1.77	$\text{C}^{\gamma}_{\text{H}_2}$ 1.74, $\text{C}^{\delta}_{\text{H}_2}$ 3.51, 3.68
Gln143	8.28	4.49	1.72, 1.90	$\text{C}^{\gamma}_{\text{H}_2}$ 2.20, $\text{N}^{\gamma}_{\text{H}_2}$ 6.72, 7.29
Cys144	9.08	4.77	2.26, 3.52	

Gln145	8.29	4.01	1.74, 2.31	$C^{\gamma}H_2$ 2.40, 2.66, $N^{\gamma}H_2$ 6.79, 7.65
His146	9.14	5.04	2.96, 4.00	H2 5.69, H4 6.60
Leu147	7.39	4.50	1.04, 1.81	$C^{\gamma}H$ 1.29, $C^{\delta}H_2$ 0.78
Cys148	8.23	5.17	2.55, 2.82	
His149	9.20	4.58	1.37, 2.37	H4 6.30
Asn150	8.82	5.15	2.69, 2.80	$N^{\beta}H_2$ 7.33, 7.43
Tyr151	8.64	4.92	3.2, 3.34	$C^{\delta}H_2$ 7.12, $C^{\epsilon}H_2$ 6.67
Val152	8.44	3.82	2.07	$C^{\gamma}H_3$ 0.88, 0.96
Gly153	7.49	3.88		
Gly154	7.44	4.19, 3.88		
Tyr155	8.25	5.69	2.78, 3.04	$C^{\delta}H_2$ 6.87, $C^{\epsilon}H_2$ 6.76
Phe156	9.05	4.76	2.95, 3.13	$C^{\delta}H_2$ 6.93, $C^{\epsilon}H_2$ 6.84
Cys157	9.16	6.11	2.80, 3.85	
Ser158	9.22	4.73	3.95, 4.26	
Cys159	9.23	5.45	2.55, 3.15	
Arg160	11.16	4.29	1.42, 1.89	$C^{\gamma}H_2$ 1.42, 1.51, $C^{\gamma}H_2$ 2.68, 2.97
Pro161	-	4.46	1.93, 2.40	$C^{\gamma}H_2$ 2.10, 2.19, $C^{\delta}H_2$ 3.64, 3.88
Gly162	9.05	3.61, 4.24		
Tyr163	8.21	4.96	2.4, 3.51	$C^{\delta}H_2$ 6.80, $C^{\epsilon}H_2$ 6.90
Glu164	9.16	4.69	1.82, 1.90	$C^{\gamma}H_2$ 2.16
Leu165	8.99	4.68	1.31, 1.78	$C^{\gamma}H$ 1.78, $C^{\delta}H_3$ 0.56, 0.77
Gln166	8.49	4.33	2.01, 2.50	$C^{\gamma}H_2$ 2.21, $N^{\gamma}H_2$ 6.83, 7.57
Glu167	8.99	4.04	2.07	$C^{\gamma}H_2$ 2.34
Asp168	7.81	4.40	2.77, 3.13	
Arg169	8.63	3.68	2.00, 2.29	$C^{\gamma}H_2$ 1.61, 1.73, $C^{\delta}H_2$ 3.18, $N^{\delta}H$ 7.14
His170	8.94	5.06	2.68, 3.45	H4 6.63
Ser171	10.39	4.61	3.88	
Cys172	8.54	5.30	1.39, 2.18	

Gln173	8.62	4.90	1.92, 2.15	$C^{\gamma}H_2$	2.32
Ala174	9.07	3.82	$C^{\beta}H_3$	1.10	
Glu175	7.91	3.89	1.78	$C^{\gamma}H_2$	1.98, 2.11

Table S2: List of hydrogen bonds occuring in more than 20% of the final structures.

Hbond donor	Hbond acceptor	occurence (number out of 19 structures)	Hbond donor	Hbond acceptor	occurence (number out of 19 structures)
123:HN	125:OD	7	150:HD21	154:O	5
123:HN	125:O	7	151:HN	154:O	16
123:HN	128:OE	6	154:HN	151:O	14
125:HN	123:O	6	156:HN	149:O	19
126:HN	124:O	6	158:HG	157:O	14
128:HN	126:O	8	158:HN	147:O	18
129:HN	150:OD1	7	160:HE	146:ND1	5
130:HN	127:O	7	160:HN	146:ND1	19
131:HG	127:O	7	163:HN	161:O	5
131:HN	127:O	8	163:HN	160:O	5
132:HH2	128:OE	8	164:HN	173:O	19
132:HN	128:O	9	166:HE	175:OE	5
132:HN	130:O	5	166:HE2	164:O	17
133:HN	131:O	6	166:HE21	175:OXT	5
134:HN	132:O	7	166:HN	171:O	19
136:HN	134:O	5	167:HN	167:OE	9
137:HN	135:O	5	169:HH	155:O	19
139:HN	137:O	9	169:HN	166:O	16
141:HE	139:OD	5	170:HE2	155:OH	7
141:HN	139:O	9	170:HN	168:OD	9
143:HN	141:O	6	170:HN	168:O	6
145:HE	172:O	11	171:HG	168:OD	10
145:HN	170:O	17	171:HN	168:OD	14
146:ND1	159:SG	6	172:HN	145:NE2	6
147:HN	158:O	14	173:HE2	175:OXT	6
149:HE2	158:OG	12	173:HN	164:O	18
149:HN	156:O	17	175:HN	173:O	10
150:HD2	127:OD	7	175:HN	162:O	7