Decoron residues that bind collagen fibril surface			*d*-band: collagen residue (name, number, chain)										*e*$_1$-band: collagen residue (name, number, chain)										*d*-band: energy of association										*e*$_1$-band: energy of association										Decoron residues that bind collagen fibril surface		
LRR	residue	number	common						wide				common						wide				common						wide				common						wide				residue	number	LRR
N-term	ILE	6	K900A										Q860B										-12.56																				ILE	6	N-term
	GLY	7	K900C	G665A																			-8.41																				GLY	7	
	GLU	9	K890B						K890B	N893B									R634A	R627B					-36.96						-29.73	-26.30									GLU	9	
	GLU	10							L891B	K890B	G892B															-34.96																GLU	10	
	GLU	14	L891B						G899A	K900C			A870A	K871A					A870A	K871A	H863B				-9.12				-9.44	19.84	-10.12										GLU	14	
	GLU	17	R894B																				-16.38																				GLU	17	
	ILE	18	R893B																																								ILE	18	
	GLU	19	R894B	K900A					R894B				H863B	K864B									-6.25	-12.98			-7.22			-21.23													GLU	19	
	PRO	20							R894B																																		PRO	20	
	MET	21	R894B						R894B										K871A						-10.66																		MET	21	
	GLY	22																	K871A																								GLY	22	
	PRO	23	R894B																R874A																								PRO	23	
	VAL	24	G902C	R894B					R894B				D873A	R874A										-8.40						8.00													VAL	24	
	CYS	25	D903C	R660B																																							CYS	25	
	PRO	26											T869B																														PRO	26	
	ARG	28	R904A																E642A				-8.38																				ARG	28	
	HIS	29							R904C																																		HIS	29	
	GLN	30	G902C	R904A					G661B	R904C			R402C						R402C						-21.65			-12.31															GLN	30	
	CYS	31	R894B						E659B	R894B													-12.62																				CYS	31	
	HIS	32	R894B						K664A				K871C										-11.10		-12.23			-4.71															HIS	32	
1	LEU	33	R894B										K871C										-6.33					-15.67															LEU	33	1
	VAL	35																	R402C																								VAL	35	
	GLN	37	G905A	R904A									R867B						R402C									-16.64			-10.23											GLN	37	
	SER	39											E876C																														SER	39	
	LYS	48							D903C																-14.62																		LYS	48	
2	ASP	58											R867B															-5.89															ASP	58	2
	GLN	60							T907C	G905C			E876C						E876A									-13.30															GLN	60	
	ASN	61							T907C				E876C																														ASN	61	
3	HIS	79							A898C				K864B															-14.84															HIS	79	3
	THR	80							D903C										K864B												-13.22												THR	80	
4	GLU	103											K871A						K871C	K864B								-23.09			-19.69	-17.65										GLU	103	4
	ARG	104							D903C																-19.04																		ARG	104	
	TYR	106							K900C																																		TYR	106	
	SER	108							E906C										E876A																								SER	108	
	LYS	109	P909A						E906C										G878A						-43.66																		LYS	109	
5	GLU	125							K900C																-44.16																		GLU	125	5
	ARG	127																	E866B												-41.67												ARG	127	
	HIS	129							R904C																-7.31																		HIS	129	
	GLU	130							R904C										G878A						-19.04						-8.86												GLU	130	
7	ARG	177																	E876A												-24.55												ARG	177	7
8	GLU	196							K900A				K864B												-28.31			-19.80															GLU	196	8
	HIS	198							K900C																																		HIS	198	
	ASP	200																	R867B												-11.17												ASP	200	
9	LYS	220	G905A	D903A						D903C									E866B					-7.75								-30.22												LYS	220	9
10	ARG	243	D903A						G899C				D873C										-24.31					5.20																ARG	243	10
	GLU	244	K900C						K900A				R867B	K871A					K871C				-33.56					-31.59	-7.27		-42.89													GLU	244	
	HIS	246																	R867B																								HIS	246	
	ASN	248											E876C						G871B	P870B								-10.31															ASN	248	
	ASN	249											E876C						G871B																								ASN	249	
11	GLN	266	K900C						R894B				K871A						K871C	G872C					-7.72			-9.10			-19.15												GLN	266	11
	TYR	269	D903C						D903C																																		TYR	269	
	ASN	272	A910A																N872B																								ASN	272	
	TRY	288																	K864B	G865B																								TRY	288	
	SER	294	R894B																																								SER	294	
12	TYR	295	R894B																				-17.64																				TYR	295	12
	SER	296	R894B	G902C					R894B				E866B						R874C	D873B			-7.42		-13.69						-10.43												SER	296	
	TYR	307	V903B						G908A	A902B			E876C	A880A					A880A	A406C																								TYR	307	
	SER	313											E866B						R874A																								SER	313	
	ARG	316																	K864B												-12.67												ARG	316	
	CYS	317																	K864B												-10.71												CYS	317	
	TYR	319																	K864B												-13.63												TYR	319	
	VAL	320	A898C										K864B																														VAL	320	
	ARG	321	D903A						D903A				D873A	E866B	K864B				D873A	D393B			-34.50		-32.67						-24.01												ARG	321	
C-term	ALA	323	R894B																				-11.82																				ALA	323	C-term
	VAL	324							R660B				K864B												-12.38			-10.61															VAL	324	
	GLN	325	R894B	R660B					R660B										R634A				-11.20	-8.45	-8.25						-13.53												GLN	325	
	LEU	326	R894B										R874A										-9.17																				LEU	326	
	GLY	327	D903C																																								GLY	327	
	TYR	329	D903C						R904C				R874A	T869B																														TYR	329	

Table S1

Principal decoron-collagen interactions. Decoron to collagen amino acid interactions are shown on the left, the matching positions (and colored highlights) on the right half of the table correspond to the calculated energy of association. Highlighted residues correspond to those that rank amongst the top 20 electrostatic pairs within one of the four conformations displayed (common and wide for the *d* and e_1 band binding sites). Although the non-highlighted residues were estimated to contribute no more than -4.5 kJ/mol (which includes the desolvation cost), they were nevertheless estimated to form persistent H-bonds and cumulatively contribute to ligand-receptor stability.