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Electronic Supplementary Information:

Energetic description of a cilengitide bound to integrin

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TABLE ES1: Residue, atomic group, interaction layer, minimal distance and MFCC binding energies between each one of the 76 amino acid residues of β-propeller and βA domains. The energy values were calculated within the GGA functional B97D.

Residue	Subunit	Ligand Atomic Group	Radius (Å)	Distance (Å)	Energy (kcal mol-1) ε=20	ε=40
Y178	α	I(C23); I(N11)H	2.0	2.17; 1.61	0.86	0.98
D218	α	I(N11)H; I(N9)H	2.0	1.99; 1.90	-13.57	-11.74
N215	β	III(C22)O5	2.0	1.85; 3.09; 3.26	2.04	1.74
Y122	β	III(C22)O5; IV(C27)H; IV(C29)H	2.5	2.69; 2.56; 2.36	-1.95	-0.50
S123	β	III(C22)O5; IV(C27)H	2.5	2.63; 2.43	-1.97	-1.84
D150	α	I(N10)H	3.0	2.89	-4.18	-2.84
F177	α	I(N10)H; I(N11)H	3.0	3.50; 2.52	0.04	-0.21
A215	α	I(C14)H; I(C16)H; I(N9)H	3.0	2.95; 3.02; 3.25	-2.28	-2.30
S121	β	III(C22)O5; III(C22)O4	3.0	2.83; 5.16	-14.23	-13.66
R214	β	III(C22)O5; III(C21)O3	3.0	2.56; 3.87	-12.26	-11.40
R216	β	II(C18)H; III(N8)H	3.0	2.70; 2.70	-2.03	-1.85
D217	β	II(C18)H; III(C19)H	3.0	3.47; 2.93	-4.43	-4.57
A218	β	II(C18)H; II(C20)O2	3.0	2.53; 2.55	-2.85	-3.02
Q180	α	I(N11)H	3.5	3.43	-1.33	-1.24
E220	β	III(C22)O4	3.5	3.06	6.28	5.07
W179	α	II(C18)H	4.5	4.02	-0.84	-0.77
T212	α	I(N11)H	4.5	4.05	-0.37	-0.38
A213	α	I(N11)H	4.5	4.48	-0.60	-0.42
Y166	β	III(C19)H	4.5	4.30	-0.39	-0.39
M180	β	IV(C29)H	4.5	4.12	-0.52	-0.52
K253	β	I(N9)H; II(N6)H	4.5	6.52; 4.32	-0.08	-0.28
D219	α	I(N9)H; I(N11)H; II(C18)H	5.0	6.64; 4.51; 5.17	-1.78	-1.29
S213	β	III(C22)O4	5.0	4.70	-0.48	-0.50
P219	β	II(C18)H; II(C20)O2	5.0	4.79; 5.82	-0.11	-0.19
A149	α	I(N10)H	5.5	5.50	-0.47	-0.39
S176	α	I(N11)H	5.5	5.49	-0.05	-0.06
K125	β	III(C22)O5; IV(C30)H	5.5	7.07; 5.40	-1.31	-0.86
V157	β	III(C22)O4	5.5	5.01	-0.07	-0.13
D251	β	III(C22)O5; IV(C27)H	5.5	5.83; 5.10	0.97	0.33
Q214	α	I(N11)H	6.0	5.52	-0.37	-0.30
F217	α	I(N11)H	6.0	5.57	0.02	-0.06
M124	β	III(C22)O5	6.0	5.66	-0.29	-0.23
D126	β	IV(C32)H	6.0	5.89	0.62	0.21
M187	β	III(C22)O5	6.0	5.90	-0.24	-0.17
A252	β	II(C20)O2; III(C17)H	6.0	5.56; 5.66	-0.28	-0.24
G151	α	I(N10)H	6.5	6.01	-0.37	-0.22
I216	α	I(N9)H	6.5	6.05	-0.05	-0.12
D119	β	III(C22)O5	6.5	6.14	1.69	0.81
Y164	β	III(C19)H	6.5	6.34	-0.06	-0.08
G181	α	I(N11)H	7.0	6.89	-0.17	-0.09
L120	β	III(C22)O4	7.0	6.80	1.01	-0.31
D158	β	III(C22)O4	7.0	6.90	0.77	0.35
P176	β	III(C22)O5	7.0	6.91	-0.22	-0.14
C177	β	III(C22)O5; IV(C29)H	7.0	6.64; 6.77	-0.16	-0.14
V212	β	III(C22)O4	7.0	6.70	-0.28	-0.20
S220	α	I(N11)H	7.5	7.31	0.08	0.03
G175	α	I(N11)H	8.0	7.62	-0.06	-0.04
T182	β	IV(C30)H	8.0	7.54	-0.05	-0.05
C184	β	III(C22)O4	8.0	7.53	-0.02	-0.04
T250	β	III(C22)O5	8.0	7.98	-0.18	-0.11
H255	β	II(C18)H	8.0	7.95	0.10	0.03
N313	β	IV(C35)O24	8.0	7.87	-0.15	-0.11
D148	α	I(N10)H	8.5	8.28	-0.53	-0.28
R211	α	I(N10)H	8.5	8.22	0.59	0.29
R248	α	I(C13)H; II(N6)H	8.5	8.49; 8.14	0.07	0.01
M165	β	III(C19)H	8.5	8.02	-0.20	-0.12
D146	α	I(N10)H	9.0	8.80	-0.82	-0.42
I147	α	I(N10)H	9.0	8.76	-0.16	-0.09
Q152	α	I(N10)H	9.0	8.77	0.04	0.01
Y221	α	I(N11)H; II(C18)H	9.0	8.78; 8.70	0.07	0.02
D127	β	III(C22)O5; IV(C27)H	9.0	9.91; 8.79	0.83	0.40
F156	β	III(C22)O5	9.0	8.74	-0.03	-0.03
P163	β	III(C19)H	9.0	8.62	-0.04	-0.03
L185	β	III(C22)O4	9.0	8.89	0.16	0.07
G153	α	I(N10)H	9.5	9.18	0.07	0.03
F154	α	II(C18)H	9.5	9.47	-0.02	-0.04
P174	α	I(N11)H	9.5	9.71	-0.12	-0.07
Q182	α	I(N11)H	9.5	9.38	0.02	0.00
R245	α	II(C18)H	9.5	9.19	0.02	-0.01
D179	β	III(C19)H; IV(C29)H; V(C36)H	9.5	9.326; 9.40; 9.33	0.32	0.14
K181	β	IV(C30)H	9.5	9.19	-0.53	-0.28
F188	β	III(C22)O4	9.5	9.14	-0.06	-0.04
G221	β	III(C19)H	9.5	9.30	0.15	0.09
P186	β	III(C22)O4	10.0	9.82	0.08	0.03
G189	β	III(C22)O4	10.0	9.80	0.05	0.02
T254	β	III(C17)H	10.0	9.55	-0.06	-0.04