

Supporting Information

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SI Text

Table S1. Contact populations between the first 7 N-terminal residues or the 11 residues of the flexible binding loop and the rest of the protein

Contact	Type	Basin 1.1	Basin 1.2	Basin 1.3	Basin 1.4
T1/L7	HO/SC	0.0	0.0	0.4	0.6
T1/Y49	HO/SC	0.6	0.0	0.0	0.0
E2/S5	HB/SC	0.0	0.0	0.5	0.2
E2/E6	WM/SC	0.0	0.0	0.6	0.7
E2/L7	HB/BB	0.0	0.0	0.7	1.0
E2/R48	SB/SC	1.0	0.0	0.0	0.0
E2/Y49	HB/BB	1.0	0.2	0.1	0.0
E2/R51	SB/SC	0.9	0.0	0.0	0.0
F3/L7	HO/SC	0.0	0.4	0.6	0.8
F3/R48	HO/SC	0.8	0.0	0.0	0.0
F3/V52	HO/SC	0.0	0.6	0.4	0.4
G4/L7	HB/BB	0.0	0.4	0.6	1.0
G4/K8	HB/BS	0.0	0.0	0.1	0.5
G4/W10	HO/SC	0.0	0.0	0.3	0.7
G4/L47	HB/BB	0.9	0.0	0.2	0.0
G4/Y49	HO/SC	0.6	0.0	0.0	0.0
S5/K8	HB/BS	0.0	0.0	0.3	0.5
S5/L47	HO/BS	0.6	0.1	0.1	0.2
E6/V69	HO/SC	0.7	0.1	0.0	0.0
L7/V52	HO/SC	0.5	0.2	0.0	0.0
L7/V66	HO/SC	0.0	0.8	0.0	0.0
L7/P67	HO/SC	0.6	0.0	0.0	0.0
L7/H68	HB/BB	1.0	0.2	0.0	0.0
L37/V43	HO/SC	0.1	0.8	0.8	0.9
P38/S41	HB/BB	0.1	0.6	0.6	0.7
L47/V52	HO/SC	0.0	0.0	0.5	0.0
L47/V69	HO/SC	0.0	0.6	0.5	0.6

Key: HO, hydrophobic; SB, salt bridge; HB, hydrogen bond; WM, water-mediated; BB, backbone/backbone; BS, backbone/side chain; SC, side chain/side chain.