

Supplementary Table 1 Interfacing residues involved in the interaction of Claudin-4

Chain A (CLDN4)	Accessible Surface Area (ASA)	Buried Surface Area (BSA)	$\Delta^{\ddagger}G$ Solvation energy effect, kcal/mol
GLY 5	37.71	2.21	-0.03
VAL 8	85.23	63.18	1.01
MET 9	67.08	21.33	0.46
ALA 12	61.26	57.02	0.75
LEU 13	12.90	9.72	0.16
VAL 15	46.67	14.74	0.24
LEU 16	25.78	17.40	0.28
GLY 37	48.62	3.44	-0.04
SER 58	109.48	0.86	-0.01
THR 59	101.23	82.41	0.62
GLY60	52.52	2.67	0.04
GLN 61	152.12	106.23	0.46
MET 62	40.69	11.12	-0.10
GLN63	49.92	44.39	0.25
CYS 64	63.11	49.01	0.53
LYS 65	81.55	33.91	-0.45
VAL 66	89.10	46.00	0.67
MET 118	84.18	8.84	0.01
ILE 119	108.22	44.65	0.69
GLY 122	26.45	17.70	0.28
VAL 123	71.70	67.17	1.06
PHE 125	71.82	38.11	0.61
LEU 126	118.34	112.16	1.74
LEU 127	59.42	50.78	0.81

GLY 129	29.57	7.64	0.12
LEU 130	72.43	28.93	0.46
VAL 132	16.05	3.69	0.06
ILE 133	84.46	48.95	0.78
TYR 165	136.07	78.97	0.67
TRP 168	189.04	74.90	1.16
ALA 169	7.19	2.35	0.04

Supplementary Table-2 Interfacing residues involved in the interaction of EphA2

Chain B (EphA2)	ASA	BSA	$\Delta^{\dagger}G$
			Solvation energy effect, kcal/mol
ASP 53	66.14	2.61	-0.03
LEU 54	59.38	3.44	-0.04
MET 55	136.85	94.14	94.14
GLN 56	114.92	24.88	24.88
ASN 57	69.20	58.66	58.66
MET 59	166.96	20.51	20.51
ASN 60	118.03	71.23	71.23
ASP 61	142.57	32.02	32.02
MET 62	141.15	0.43	0.43
ILE 64	66.34	30.46	30.46
MET 66	75.40	69.40	69.40
SER 68	17.42	0.96	0.96
LYS 99	62.51	16.07	0.26
THR 101	20.19	19.07	0.19
ARG 103	102.34	72.75	-2.49
ASP 104	39.14	31.15	0.41
ASN 106	145.32	44.86	0.30

SER 107	21.15	4.15	0.06
PHE 108	24.29	1.25	0.02
PRO 109	130.59	29.03	0.46
GLU 117	73.02	12.22	0.01
PRO 147	30.54	6.85	0.11
ASP 148	147.30	30.07	-0.30
HIS 160	162.44	152.42	0.43
VAL 161	91.60	74.71	0.50
LYS 162	88.62	69.89	0.89
LEU 163	123.28	106.04	1.40
ASN164	12.61	0.17	0.00
VAL 165	97.58	23.76	0.38
ALA 190	36.67	21.02	0.34
LEU 192	69.82	45.45	0.73
SER 193	54.04	0.49	-0.01