

**Table 1S:** The docking results of FIL with  $\beta$ -actin (PDB:1HLU)Receptor ( $\beta$ -actin) interface residue(s):

ILE	34a	4.640
ARG	37a	3.936
ARG	39a	2.686
HIS	40a	3.529
GLN	41a	3.619
ARG	62a	4.459
LEU	65a	4.423
THR	66a	2.428
LEU	67a	0.830
LYS	68a	2.986
TYR	69a	2.528
ARG	183a	3.308
ASP	184a	3.663
ASP	187a	1.972
TYR	188a	2.245
LYS	191a	2.837
THR	194a	3.147
GLU	195a	1.061
ARG	196a	3.534
GLY	197a	3.530
ARG	206a	4.076
PHE	223a	4.167
MET	227a	1.980
ASN	252a	2.323
ARG	256a	2.302
SER	265a	3.924
PHE	266a	2.311
LEU	267a	2.553
GLY	268a	2.903
MET	269a	4.415
GLU	270a	2.974

## Ligand (FIL) interface residue(s):

ACE	4A	3.619
GLY	5A	3.936
PRO	45A	4.527
GLU	46A	2.604
VAL	49A	2.647
LEU	50A	1.980
HIS	53A	2.245
GLY	56A	3.924
ILE	57A	3.744
PRO	58A	2.903
TRP	59A	2.553
ALA	60A	4.491
PRO	61A	3.580
LEU	62A	3.747
SER	63A	1.972
SER	64A	3.483
PRO	66A	4.099
SER	67A	0.830
GLN	68A	2.705
ALA	69A	2.428
LEU	70A	4.496
GLN	71A	4.142
TYR	86A	4.076
GLN	135A	3.194
GLY	136A	3.249
ALA	137A	2.974
LEU	153A	4.336
SER	156A	4.426
HIS	157A	1.061
SER	160A	3.147
GLU	163A	4.874
HIS	171A	2.825
LEU	172A	2.686
ALA	173A	4.749
GLN	174A	3.186
PRO	175A	3.127

**Table 1** FIL with  $\beta$ -actin interface residues

34a - 67A	4.640	191a - 86A	4.076
37a - 4A	3.977	191a - 157A	3.400
37a - 5A	3.936	191a - 160A	4.480
39a - 69A	3.272	194a - 160A	3.147
39a - 171A	2.825	194a - 163A	4.874
39a - 172A	2.686	195a - 45A	4.527
39a - 173A	4.749	195a - 46A	2.604
39a - 174A	3.186	195a - 49A	4.868
39a - 175A	3.127	195a - 153A	4.336
40a - 174A	4.723	195a - 156A	4.426
40a - 175A	3.529	195a - 157A	1.061
41a - 4A	3.619	195a - 160A	4.444
41a - 5A	4.499	196a - 46A	3.534
62a - 66A	4.585	197a - 46A	3.530
62a - 67A	4.459	206a - 63A	4.076
65a - 66A	4.423	206a - 66A	4.832
66a - 67A	4.493	223a - 53A	4.167
66a - 68A	3.195	227a - 50A	1.980
66a - 69A	2.428	252a - 49A	4.121
66a - 70A	4.496	252a - 50A	2.323
66a - 171A	3.663	256a - 49A	2.647
67a - 66A	4.099	256a - 50A	4.387
67a - 67A	0.830	256a - 53A	2.302
67a - 68A	2.705	265a - 56A	3.924
68a - 67A	2.986	265a - 57A	4.794
68a - 68A	4.512	265a - 58A	4.410
68a - 71A	4.142	266a - 53A	2.311
69a - 67A	2.528	266a - 57A	3.744
69a - 68A	4.695	266a - 58A	4.209
183a - 63A	3.308	266a - 59A	4.115
183a - 64A	3.483	267a - 58A	4.049
184a - 59A	3.663	267a - 59A	2.553
184a - 63A	4.931	268a - 58A	2.903
187a - 59A	3.683	268a - 59A	4.196
187a - 61A	3.580	268a - 136A	3.979
187a - 62A	3.747	268a - 137A	3.583
187a - 63A	1.972	269a - 59A	4.415
188a - 53A	2.245	269a - 137A	4.808
188a - 59A	3.494	270a - 135A	3.194
191a - 58A	4.342	270a - 136A	3.249
191a - 59A	2.837	270a - 137A	2.974
191a - 60A	4.491		

**Table 2S:** The docking results of FIL with S100-A9 (PDB: 4GGF)

Receptor (S100-A9) interface residue(s):

LEU	8A	4.150
HIS	61A	2.777
ASP	65A	2.781
LEU	66A	2.860
ASP	67A	4.937
THR	68A	3.310
MET	81A	2.660
ALA	84A	2.563
ARG	85A	3.228
THR	87A	3.827
TRP	88A	2.466
HIS	91A	3.020
GLU	92A	2.116
MET	94A	3.048
HIS	95A	2.706
GLU	96A	3.157
GLY	97A	4.984
GLU	99A	4.102
HIS	103A	4.587

Ligand (FIL) interfaces residue(s):

HIS	44A	4.166
GLU	46A	4.150
VAL	49A	3.983
HIS	53A	3.157
ILE	57A	3.430
PRO	58A	4.063
TRP	59A	2.116
ALA	60A	3.921
PRO	61A	3.611
LEU	62A	3.053
SER	63A	4.288
TYR	86A	4.168
HIS	157A	3.020
SER	160A	3.130
PHE	161A	3.606
GLU	163A	2.563
VAL	164A	2.466
ARG	167A	2.660
ARG	170A	3.310
HIS	171A	2.777

**Table 2.** FIL with S100-A9 interface residue pairs

8A - 44A	4.166	88A - 164A	2.466
8A - 46A	4.150	91A - 59A	3.998
61A - 171A	2.777	91A - 60A	4.713
65A - 167A	2.781	91A - 86A	4.168
65A - 170A	4.672	91A - 157A	3.020
65A - 171A	4.136	91A - 160A	4.336
66A - 167A	2.860	92A - 59A	2.116
67A - 167A	4.937	92A - 60A	4.171
68A - 167A	4.716	92A - 61A	3.793
68A - 170A	3.310	92A - 62A	4.997
81A - 167A	2.660	94A - 49A	3.983
81A - 170A	4.413	94A - 53A	3.199
84A - 163A	2.563	94A - 157A	3.048
85A - 164A	4.599	95A - 53A	3.207
85A - 167A	3.228	95A - 57A	3.430
87A - 160A	3.827	95A - 58A	4.063
87A - 163A	4.979	95A - 59A	2.706
88A - 60A	3.921	95A - 157A	4.273
88A - 61A	3.611	96A - 53A	3.157
88A - 62A	3.053	97A - 53A	4.984
88A - 63A	4.288	99A - 53A	4.102
88A - 160A	3.130	103A - 59A	4.587
88A - 161A	3.606		

**Table 3S.** The docking results of FIL with CD3 receptor (PDB:1XIW)

Receptor (CD3) interface residue(s):

LEU	39a	3.471
LEU	46a	4.190
THR	47a	4.133
PHE	50a	2.795
LEU	51a	4.908
VAL	53a	3.992
LYS	54a	2.448
LEU	144f	4.952
LEU	147f	3.415
VAL	148f	2.091
TYR	150f	4.716
TRP	151f	1.220
SER	152f	4.718
ASN	154f	3.950
ARG	155f	3.298
LEU	119	3.927
	g	
PHE	120	3.327
	g	
ILE	123	1.529
	g	
VAL	124	3.947
	g	
ILE	126	4.513
	g	
PHE	127	2.293
	g	
VAL	128	4.199
	g	
ALA	130	2.629
	g	
VAL	131	2.404
	g	
GLY	132	4.346
	g	
VAL	133	4.945
	g	
TYR	134	2.930
	g	
PHE	135	3.177
	g	

Ligand (FIL) interfaces residue(s):

VAL	22A	4.577
ARG	23A	4.150
GLN	26A	1.220
ALA	30A	4.930
GLN	33A	3.177
THR	39A	3.846
TYR	40A	2.448
LYS	41A	3.992
LEU	42A	2.932
PRO	45A	3.757
GLU	46A	4.134
GLU	47A	4.190
VAL	49A	4.199
LEU	50A	3.471
HIS	53A	3.810
ILE	57A	4.959
TRP	59A	1.529
ALA	60A	3.191
PRO	61A	3.847
LEU	62A	4.314
SER	63A	4.820
TYR	86A	3.238
PHE	145A	3.276
ARG	148A	2.875
SER	156A	2.404
HIS	157A	4.112
GLN	159A	3.480
SER	160A	2.293
PHE	161A	3.215
LEU	162A	4.196
GLU	163A	2.091
VAL	164A	4.617
TYR	166A	2.731
ARG	167A	3.415
ARG	170A	3.902

**Table 3.** FIL with CD3 interface residue pairs

39a - 50A	3.471	123g - 62A	4.314
46a - 47A	4.190	124g - 59A	3.947
47a - 145A	4.133	124g - 157A	4.849
50a - 40A	2.795	126g - 160A	4.513
50a - 41A	4.029	127g - 59A	4.530
50a - 42A	2.932	127g - 60A	3.191
50a - 145A	3.276	127g - 86A	3.238
51a - 145A	4.908	127g - 156A	4.591
53a - 41A	3.992	127g - 157A	4.112
54a - 39A	3.846	127g - 160A	2.293
54a - 40A	2.448	127g - 161A	3.215
54a - 148A	2.875	127g - 164A	4.617
144f - 164A	4.952	128g - 46A	4.600
147f - 167A	3.415	128g - 49A	4.199
148f - 163A	2.091	128g - 160A	4.395
148f - 164A	4.635	130g - 160A	3.418
148f - 167A	4.580	130g - 163A	2.629
150f - 167A	4.716	131g - 33A	4.842
151f - 22A	4.577	131g - 45A	3.757
151f - 26A	1.220	131g - 46A	4.134
151f - 162A	4.196	131g - 156A	2.404
151f - 163A	2.809	131g - 157A	4.398
151f - 166A	2.731	131g - 159A	4.145
151f - 167A	3.485	131g - 160A	2.632
151f - 170A	3.902	131g - 163A	4.051
152f - 163A	4.718	132g - 46A	4.346
154f - 170A	3.950	133g - 163A	4.945
155f - 23A	4.150	134g - 26A	3.813
155f - 166A	3.298	134g - 30A	4.930
155f - 170A	4.543	134g - 159A	3.480
119g - 59A	3.927	134g - 163A	2.930
119g - 63A	4.820	135g - 33A	3.177
120g - 53A	3.810	135g - 45A	4.368
120g - 57A	4.959		
120g - 59A	3.327		
123g - 59A	1.529		
123g - 60A	3.818		
123g - 61A	3.847		

**Table 4S.** The docking results of FIL with CD20 (PDB: 3PP4).

<u>Receptor (CD20) interface residue(s):</u>			<u>Ligand (FIL) interface residue(s):</u>		
ILE	80A	3.334	HIS	53A	2.754
THR	83A	3.042	ILE	57A	4.438
VAL	84A	2.189	TRP	59A	2.661
TRP	85A	2.542	ALA	60A	4.180
TYR	86A	4.872	PRO	61A	3.442
TRP	89A	2.422	LEU	62A	3.444
GLY	90A	4.307	SER	63A	2.422
ILE	92A	4.084	SER	64A	3.080
MET	93A	3.184	CYS	65A	4.578
ILE	95A	2.754	PRO	66A	2.933
ILE	96A	2.940	SER	67A	2.785
SER	99A	4.430	GLN	78A	3.403
MET	119A	4.579	SER	160A	4.732
LEU	122A	2.661	GLU	163A	3.431
PHE	125A	3.080	VAL	164A	2.189
ALA	126A	3.871	TYR	166A	4.739
SER	129A	2.811	ARG	167A	2.686
ILE	132A	3.847	VAL	168A	4.274
LEU	133A	3.118	ARG	170A	2.685
MET	136A	2.785	HIS	171A	3.270
LEU	147A	3.270			
LYS	148A	3.786			
MET	149A	3.437			
GLU	150A	2.915			
SER	151A	2.686			
LEU	152A	3.568			
ASN	153A	2.685			
PHE	154A	3.657			

**Table 4 .** FIL with CD20 interface residue pairs

---

80A - 66A	3.334
83A - 163A	4.915
83A - 164A	4.082
83A - 167A	3.042
83A - 168A	4.926
84A - 62A	4.918
84A - 65A	4.578
84A - 66A	2.933
84A - 164A	2.189
84A - 168A	4.274
85A - 160A	4.732
85A - 163A	3.431
85A - 164A	2.542
85A - 167A	4.506
86A - 63A	4.872
89A - 59A	3.020
89A - 60A	4.180
89A - 61A	3.442
89A - 62A	3.444
89A - 63A	2.422
89A - 164A	4.837
90A - 59A	4.307
92A - 53A	4.084
92A - 59A	4.584
93A - 59A	3.184
95A - 53A	2.754
96A - 53A	2.940
96A - 57A	4.438
96A - 59A	4.437
99A - 53A	4.430
119A - 59A	4.579
122A - 59A	2.661
125A - 61A	4.827
125A - 63A	3.105
125A - 64A	3.080
125A - 78A	3.403
126A - 63A	3.871
129A - 63A	2.811
129A - 64A	4.666
132A - 67A	3.847
133A - 63A	3.998
133A - 66A	3.118
133A - 67A	3.736
136A - 66A	3.758
136A - 67A	2.785
147A - 66A	4.725
147A - 171A	3.270
148A - 171A	3.786
149A - 66A	4.613
149A - 167A	4.437
149A - 168A	4.905
149A - 171A	3.437
150A - 167A	2.915
151A - 167A	2.686
152A - 163A	4.645
152A - 167A	3.568
153A - 166A	4.739
153A - 167A	3.471
153A - 170A	2.685
154A - 163A	3.657

---