1 Supplementary information

#	bound	unbound	$L_{receptor}$	$L_{peptide}$	$Best_{400}$	$Best_{10Clust.}$
1	1awr A:G	2alf A	164	6	2.22	2.22
2	1cka A:B	2dvj A	57	9	4.15	4.60
3	1d4t A:B	1d1z A	104	11	5.00	7.57
4	1ddv A:B	1i2h A	104	6	1.83	6.36
5	1eg4 A:P	1eg3 A	260	13	6.87	13.21
6	1er8 E:I	1oew A	330	8	2.59	2.60
7	1gyb A:E	1gy7 A	122	5	5.51	8.57
8	1hc9 A:C	2abx A	74	13	7.27	10.66
9	1jbu H:X	2bz6 H	239	15	6.10	6.73
10	1jwg A:C	1jwf A	140	5	2.27	2.28
11	1kl3 A:E	2rtm A	120	6	6.11	6.11
12	1lvm A:E	1lvb A	229	7	2.53	2.53
13	1mfg A:B	2h3l A	95	9	5.41	8.87
14	1n7f A:C	1n7e A	86	8	1.05	1.05
15	1nq7 A:B	1n83 A	244	10	0.75	0.75
16	1nvr A:B	2qhn A	264	5	0.75	0.76
17	1nx1 A:C	1alv A	173	11	1.21	1.22
18	1oai A:B	1go5 A	59	9	4.43	5.08
19	1ou8 A:C	1ou9 B	106	8	3.80	3.80
20	1rxz A:B	1rwz A	245	11	5.86	6.73
21	1sfi A:I	1utn A	223	14	5.20	8.12
22	1ssh A:B	1oot A	60	11	3.96	5.98
23	1t4f M:P	1z1m A	88	9	2.83	3.32
24	1t7r A:B	2am9 A	250	10	2.29	4.78
25	1tp5 A:B	1tq3 A	115	6	1.33	1.34
26	1w9e A:R	1r6j A	164	5	1.35	1.35
27	1x2r A:B	1x2j A	290	9	3.67	6.91
28	1ywo A:P	1y0m A	55	10	2.98	5.45
29	1z9o A:G	1z9l A	238	9	4.36	6.95
30	2ak5 B:D	2g6f X	64	8	2.80	4.90
31	2b9h A:C	2b9f A	337	12	3.10	3.11
32	2c3i B:A	2j2i B	266	8	2.79	3.33
33	2cch B:E	1h1r A	256	12	2.44	3.80
34	2ds8 A:Q	2ds7 A	41	6	1.08	1.08
35	2fgr A:B	2fgq X	332	8	5.57	16.04
36	2fmf A:B	1jbe A	128	13	4.94	5.87
37	2fnt A:P	3hau A	198	7	2.26	2.27
38	2foj A:B	2f1w A	137	7	2.12	5.90
39	2h9m A:B	2h14 A	304	5	1.37	1.37
40	2ho2 A:B	2e45 A	33	10	3.56	10.63
41	2hpl A:B	2hpj A	100	5	2.44	2.97
42	2ipu K:P	1yej H	442	7	3.86	8.34
43	2j6f A:C	2j6k A	57	8	3.18	4.62
44	2o02 A:P	3rdh A	224	14	4.95	6.35
45	2o9v A:B	2o9s A	67	10	3.87	4.73
46	2puy B:E	2yql A	60	10	2.80	2.80
47	2qos C:A	1lf7 A	173	11	5.45	7.13
48	2r7g A:B	3pom A	337	10	2.76	2.77
49	2vj0 A:Q	1b9k A	246	8	3.29	14.53
50	2zjd A:B	1v49 A	121	10	2.70	2.97
51	3bu3 A:B	3ekk A	297	14	5.14	10.54
52	3d1e A:P	3d1g A	366	6	2.39	7.27
53	3d9t A:C	2qbh AC	95	6	4.17	5.94
54	1elw A:C	1a17 A	107	8	2.38	2.76
55	1ntv A:B	1p3r A	148	10	3.12	3.12
56	1u00 A:P	2v7y A	143	9	2.85	2.85
57	1ymt A:B	1pk5 A	242	10	1.34	1.35
58	2iv9 B:P	-	466	9	3.81	4.98
59	2jam A:D	3dxn A	258	6	3.60	3.60
60	2p0w A:P	1bob A	306	15	6.98	13.71
61	2p1k A:C	1pwj A	89	11	6.04	7.12
Mean				9	3.48	5.32

Table 1: Targets and results. For each target, the protein data bank identifiers and chain labels are reported for the bound and unbound conformation, together with the size of the receptor sequence (unbound) ($L_{receptor}$), the size of the peptide ($L_{peptide}$). $Best_{400}$ denotes the best peptide RMSd without superimposition to the experimental peptide pose, among the 400 peptide-protein complexes generated using the protein unbound conformation. $Best_{10Clust.}$ denotes the best peptide RMSd without superimposition among the poses of the 10 clusters of lowest energy. Peptides 54 to 61 have not been considered in the CABS-dock benchmark. For the bound conformation the chain labels of the receptor and the peptide are separated by a colon.