Supplementary Table R3-Q3-1. Calculation of the prediction ratio for the scores of the docking poses

The prediction ratio (p_{δ}^{error}) is defined in *Marillet et al.* (reference) as the percentage of cases such that the difference between the experimental and predicted free energies is equal or smaller than a specified amount δ. We have calculated the prediction ratio for the standard cases of δ equal to 1.4, 2.8, and 4.2 Kcal/mol. We have also added the absolute number of predictions for each prediction ratio in the column *abs*. We have used the scores of the native conformation of the complexes and also the averages with all the poses from a docking search with PatchDock. Several scores are used, some taken from our analysis and others from the CCHarPPI server.

	δ (Kcal/mol)	AB2				AB2 Rigid				AB2 Flexible			
		Native		All decoys		Native		All decoys		Native		All decoys	
		%	abs	%	abs	%	abs	%	abs	%	abs	%	abs
FiberDock	$\delta \leq 1.4$	38.30	36	39.36	37	29.17	14	29.17	14	47.83	22	50.00	23
	$1.4 < \delta \leq 2.8$	29.79	28	31.91	30	27.08	13	35.42	17	32.61	15	28.26	13
	$2.8 < \delta \leq 4.2$	17.02	16	14.89	14	31.25	15	20.83	10	2.17	1	8.70	4
	$\delta > 4.2$	14.89	14	13.83	13	12.50	6	14.58	7	17.39	8	13.04	6
aVdW	$\delta \leq 1.4$	41.49	39	36.17	34	35.42	17	33.33	16	47.83	22	39.13	18
	$1.4 < \delta \leq 2.8$	25.53	24	28.72	27	25.00	12	22.92	11	26.09	12	34.78	16
	$2.8 < \delta \leq 4.2$	20.21	19	20.21	19	27.08	13	27.08	13	13.04	6	13.04	6
	$\delta > 4.2$	12.77	12	14.89	14	12.50	6	16.67	8	13.04	6	13.04	6
rVdW	$\delta \leq 1.4$	38.30	36	35.11	33	33.33	16	31.25	15	43.48	20	39.13	18
	$1.4 < \delta \leq 2.8$	20.21	19	29.79	28	12.50	6	22.92	11	28.26	13	36.96	17
	$2.8 < \delta \leq 4.2$	23.40	22	18.09	17	33.33	16	25.00	12	13.04	6	10.87	5
	$\delta > 4.2$	18.09	17	17.02	16	20.83	10	20.83	10	15.22	7	13.04	6
aElec	$\delta \leq 1.4$	37.23	35	41.49	39	33.33	16	33.33	16	41.30	19	50.00	23
	$1.4 < \delta \leq 2.8$	24.47	23	28.72	27	18.75	9	29.17	14	30.43	14	28.26	13
	$2.8 < \delta \leq 4.2$	19.15	18	13.83	13	25.00	12	22.92	11	13.04	6	4.35	2
	$\delta > 4.2$	19.15	18	15.96	15	22.92	11	14.58	7	15.22	7	17.39	8
rElec	$\delta \leq 1.4$	37.23	35	39.36	37	35.42	17	29.17	14	39.13	18	50.00	23
	$1.4 < \delta \leq 2.8$	23.40	22	29.79	28	14.58	7	31.25	15	32.61	15	28.26	13
	$2.8 < \delta \leq 4.2$	21.28	20	14.89	14	29.17	14	25.00	12	13.04	6	4.35	2
	$\delta > 4.2$	18.09	17	15.96	15	20.83	10	14.58	7	15.22	7	17.39	8
laElec	$\delta \leq 1.4$	37.23	35	42.55	40	33.33	16	35.42	17	41.30	19	50.00	23
	$1.4 < \delta \leq 2.8$	23.40	22	26.60	25	18.75	9	27.08	13	28.26	13	26.09	12
	$2.8 < \delta \leq 4.2$	21.28	20	15.96	15	27.08	13	22.92	11	15.22	7	8.70	4
	$\delta > 4.2$	18.09	17	14.89	14	20.83	10	14.58	7	15.22	7	15.22	7
lrElec	$\delta \leq 1.4$	38.30	36	41.49	39	33.33	16	33.33	16	43.48	20	50.00	23
	$1.4 < \delta \leq 2.8$	18.09	17	28.72	27	12.50	6	29.17	14	23.91	11	28.26	13
	$2.8 < \delta \leq 4.2$	25.53	24	14.89	14	33.33	16	22.92	11	17.39	8	6.52	3
	$\delta > 4.2$	18.09	17	14.89	14	20.83	10	14.58	7	15.22	7	15.22	7
HB	$\delta \leq 1.4$	37.23	35	38.30	36	31.25	15	33.33	16	43.48	20	43.48	20
	$1.4 < \delta \leq 2.8$	29.79	28	19.15	18	29.17	14	12.50	6	30.43	14	26.09	12
	$2.8 < \delta \leq 4.2$	15.96	15	25.53	24	16.67	8	35.42	17	15.22	7	15.22	7
	$\delta > 4.2$	17.02	16	17.02	16	22.92	11	18.75	9	10.87	5	15.22	7
EPAIR	$\delta \leq 1.4$	32.98	31	41.49	39	29.17	14	35.42	17	36.96	17	47.83	22
	$1.4 < \delta \leq 2.8$	29.79	28	26.60	25	20.83	10	27.08	13	39.13	18	26.09	12
	$2.8 < \delta \leq 4.2$	19.15	18	15.96	15	29.17	14	16.67	8	8.70	4	15.22	7
	$\delta > 4.2$	18.09	17	15.96	15	20.83	10	20.83	10	15.22	7	10.87	5
ES3DC	$\delta \leq 1.4$	38.30	36	46.81	44	33.33	16	39.58	19	43.48	20	54.35	25
	$1.4 < \delta \leq 2.8$	27.66	26	26.60	25	22.92	11	31.25	15	32.61	15	21.74	10
	$2.8 < \delta \leq 4.2$	19.15	18	9.57	9	27.08	13	10.42	5	10.87	5	8.70	4
	$\delta > 4.2$	14.89	14	17.02	16	16.67	8	18.75	9	13.04	6	15.22	7
E3D	$\delta \leq 1.4$	36.17	34	38.30	36	33.33	16	31.25	15	39.13	18	45.65	21
	$1.4 < \delta \leq 2.8$	30.85	29	20.21	19	25.00	12	16.67	8	36.96	17	23.91	11
	$2.8 < \delta \leq 4.2$	20.21	19	24.47	23	29.17	14	31.25	15	10.87	5	17.39	8
	$\delta > 4.2$	12.77	12	17.02	16	12.50	6	20.83	10	13.04	6	13.04	6

ZRANK	$\delta \leq 1.4$	38.30	36	-	-	35.42	17	-	-	41.30	19	-	-
	$1.4 < \delta \leq 2.8$	25.53	24	-	-	16.67	8	-	-	34.78	16	-	-
	$2.8 < \delta \leq 4.2$	22.34	21	-	-	33.33	16	-	-	10.87	5	-	-
	$\delta > 4.2$	13.83	13	-	-	14.58	7	-	-	13.04	6	-	-
ZRANK2	$\delta \leq 1.4$	38.30	36	-	-	35.42	17	-	-	41.30	19	-	-
	$1.4 < \delta \leq 2.8$	22.34	21	-	-	16.67	8	-	-	28.26	13	-	-
	$2.8 < \delta \leq 4.2$	24.47	23	-	-	31.25	15	-	-	17.39	8	-	-
	$\delta > 4.2$	14.89	14	-	-	16.67	8	-	-	13.04	6	-	-
RosettaDock	$\delta \leq 1.4$	37.23	35	-	-	33.33	16	-	-	41.30	19	-	-
	$1.4 < \delta \leq 2.8$	29.79	28	-	-	27.08	13	-	-	32.61	15	-	-
	$2.8 < \delta \leq 4.2$	17.02	16	-	-	20.83	10	-	-	13.04	6	-	-
	$\delta > 4.2$	15.96	15	-	-	18.75	9	-	-	13.04	6	-	-
PyDock	$\delta \leq 1.4$	38.30	36	-	-	29.17	14	-	-	47.83	22	-	-
	$1.4 < \delta \leq 2.8$	22.34	21	-	-	22.92	11	-	-	21.74	10	-	-
	$2.8 < \delta \leq 4.2$	25.53	24	-	-	35.42	17	-	-	15.22	7	-	-
	$\delta > 4.2$	13.83	13	-	-	12.50	6	-	-	15.22	7	-	-
PISA	$\delta \leq 1.4$	35.11	33	-	-	25.00	12	-	-	45.65	21	-	-
	$1.4 < \delta \leq 2.8$	30.85	29	-	-	33.33	16	-	-	28.26	13	-	-
	$2.8 < \delta \leq 4.2$	21.28	20	-	-	33.33	16	-	-	8.70	4	-	-
	$\delta > 4.2$	12.77	12	-	-	8.33	4	-	-	17.39	8	-	-
PIE	$\delta \leq 1.4$	41.49	39	-	-	33.33	16	-	-	50.00	23	-	-
	$1.4 < \delta \leq 2.8$	23.40	22	-	-	22.92	11	-	-	23.91	11	-	-
	$2.8 < \delta \leq 4.2$	19.15	18	-	-	29.17	14	-	-	8.70	4	-	-
	$\delta > 4.2$	15.96	15	-	-	14.58	7	-	-	17.39	8	-	-
SIPPER	$\delta \leq 1.4$	41.49	39	-	-	31.25	15	-	-	52.17	24	-	-
	$1.4 < \delta \leq 2.8$	22.34	21	-	-	25.00	12	-	-	19.57	9	-	-
	$2.8 < \delta \leq 4.2$	20.21	19	-	-	25.00	12	-	-	15.22	7	-	-
	$\delta > 4.2$	15.96	15	-	-	18.75	9	-	-	13.04	6	-	-