

Supplementary Information Table S1

Root Mean Square Deviations. When several structures are compared the average rms is shown.

FREE vs Protein/Protein Complex				
Free	ChID	Complex	CHID	rms (CA)
1f46	A	1f47	B	0,90
1z1m	A	1ycq	A	1,80
1z1m	A	1ycr	A	1,90
1r2d	A	1bxl	A	2,3
1f9x	A	1g73	C	2,30
1f9x	A	1nw9	A	2,40

FREE vs Protein/Inhibitor Complex				
Free	ChID	Protein/Inhibitor	CHID	rms (CA)
1f46	A	1s1j,1s1s,1y2f,1y2g	A (1s1s:B)	0,70
1z1m	A	1rv1,1t4e	A	2,05
1r2d	A	1ysg,1ysi,1ysn,2o1y,2o2m, 2o2n,2yxj	A	1,79
1f9x	A	2jk7,2opy,3clx,3cm7,3cm2,3eyl	A	2,62
1f9x	A	1tfq,1tft	A	2,40

Protein/Protein vs Protein/Inhibitor Complexes				
Complex	CHID	Protein/Inhibitor	CHID	rms (CA)
1F47	B	1s1j,1s1s,1y2f,1y2g	A (1s1s:B)	0,85
1YCQ	A	1ttv	A	1,10
1YCR	A	1rv1,1t4e	A	0,95
1BXL	A	1ysg,1ysi,1ysn,2o1y,2o2m, 2o2n,2yxj	A	2,93
1G73	C	2jk7,2opy,3clx,3cm7,3cm2,3eyl	A	0,52
1NW9	A	1tfq,1tft	A	2,10

1scn	E	1cse	E	0,30
1scn	E	1r0r	E	0,30
1sup	A	1to2	E	0,30
1hj9	A	2uuy	A	0,70
2zff	H	3b9f	H	0,60
1r6k	A	1tue	B	1,40
2cio	A	3e1z	B	0,40
1m47	A	1z92	A	1,30
na		1oo9	A	
2ppn	A	1b6c	A	0,50
na		2j0t	A	

1scn	E	1bh6	A	0,40
1scn	E	1bh6	A	0,40
1sup	A	1bh6	A	0,50
1hj9	A	2fs8	A	1,60
2zff	H	1jwt	A	0,40
1r6k	A	1r6n	A	0,90
2cio	A	1cvz	A	0,30
1m47	A	1m48	A	0,60
na		1usn	A	
2ppn		1j4r	A	
na		966c	A	

1cse	E	1bh6	A	0,40
1r0r	E	1bh6	A	0,40
1to2	E	1bh6	A	0,50
2uuy	A	2fs8	A	1,50
3b9f	H	1jwt	A	0,90
1tue	B	1r6n	A	1,50
3e1z	B	1cvz	A	0,40
1z92	A	1m48	A	1,40
1oo9	A	1usn	A	1,20
1b6c	A	1j4r	A	0,61
2j0t	A	966c	A	0,50

Class I	Mean	1,86
	Stdev	0,59414
Class II	Mean	0,64
	Stdev	0,42459
ALL	Mean	1,08
	Stdev	0,76478

Class I	Mean	1,91
	Stdev	0,7481
Class II	Mean	0,64
	Stdev	0,43074
ALL	Mean	1,13
	Stdev	0,84278

Class I	Mean	1,41
	Stdev	0,91668
Class II	Mean	0,85
	Stdev	0,46717
ALL	Mean	1,04
	Stdev	0,6895