

Table 1. Protein-protein complexes

Code	Complex	Res (Å)	Interface area B (Å ²)	H-bonds N _{hb}	Water molecules N _{wat} ^a	Reference
A. Protease-inhibitor (19)						
2ptc	Trypsin-PTI	1.9	1430	12	18	Huber <i>et al.</i> (1974)
1avw	Trypsin-soybean inhibitor	1.8	1740	11	12	Song & Suh (1998)
1mct	Trypsin-bitter gourd inhibitor	1.6	1520	10	13	Huang <i>et al.</i> (1993)
3tpi	Trypsinogen-PTI	1.9	1420	11	17	Marquart <i>et al.</i> (1983)
1tgs	Trypsinogen-PSTI	1.8	1730	10	18	Bolognesi <i>et al.</i> (1982)
1cho	Chymotrypsin-ovomucoid	1.8	1470	10	17	Fujinaga <i>et al.</i> (1987)
1acb	Chymotrypsin-eglin C	2.0	1540	9	7	Frigerio <i>et al.</i> (1992)
1cbw	Chymotrypsin-PTI	2.6	1460	9		Scheidig <i>et al.</i> (1997)
1ppf	Elastase-ovomucoid	1.8	1330	6	18	Bode <i>et al.</i> (1986)
1fle	Elastase-elafin	1.9	1780	9	11	Tsunemi <i>et al.</i> (1996)
2kai	Kallikrein-PTI	2.5	1440	10		Chen & Bode (1983)
1hia	Kallikrein-hirustatin	2.4	1740	10	14	Mittl <i>et al.</i> (1997)
3sgb	S. griseus protease B-ovomucoid	1.8	1280	8	16	Read <i>et al.</i> (1983)
1mkw	Thrombin-prethrombin	2.3	1280	14	6	Malkowski <i>et al.</i> (1997)
1cse	Subtilisin-eglin C	1.2	1490	12	23	Bode <i>et al.</i> (1987)
2sic	Subtilisin-SSI	1.8	1620	10	20	Takeuchi <i>et al.</i> (1991)
2sni	Subtilisin-Cl2	2.1	1630	10	10	McPhalen & James (1987)
1stf	Papain-stefin	2.4	1790	5	13	Stubbs <i>et al.</i> (1990)
4cpa	Carboxypeptidase A-inhibitor	2.5	1360	5		Rees & Lipscomb (1982)
B. Large protease complexes (5)						
1bth	Thrombin E192Q-PTI	2.3	2380	13	5	van de Locht <i>et al.</i> (1997)
4htc	Thrombin-hirudin	2.3	3350	16	38	Rydel <i>et al.</i> (1991)
1tbq	Thrombin-rhodniin	3.1	3510	12		van de Locht <i>et al.</i> (1995)
1toc	Thrombin-ornithodorin	3.1	3510	15		van de Locht <i>et al.</i> (1996)
1dan	Factor VIIA-soluble tissue factor	2.0	3770	23	28	Banner <i>et al.</i> (1996)
C. Antibody-antigen (19)						
1vfb	Fv D1.3-lysozyme	1.8	1400	9	28	Bhat <i>et al.</i> (1994)
1mlc	Fab D44.1- lysozyme	2.1	1410	5	7	Braden <i>et al.</i> (1994)
1jhl	Fv D11.15-lysozyme	2.4	1260	5		Chitarra <i>et al.</i> (1993)
3hfl	Fab Hy-HEL5-lysozyme	2.7	1730	11		Sheriff <i>et al.</i> (1987)
3hfm	Fab Hy-HEL10-lysozyme	3.0	1610	11		Padlan <i>et al.</i> (1989)
1fbi	Fab 9.13.7-lysozyme	3.0	1720	12		Lescar <i>et al.</i> (1995)
1mel	Camel H chain-lysozyme	2.5	1710	8		Desmyter <i>et al.</i> (1996)
1jel	Fab Jel42-HPR	2.8	1360	5		Prasad <i>et al.</i> (1993)
1nsn	Fab N10-Staph. nuclease	2.9	1800	4		Bossart-Whitaker <i>et al.</i> (1995)
1osp	Fab-Borrelia OSP-A	2.0	1500	7	27	Li <i>et al.</i> (1997)
1nca	Fab NC41-flu neuraminidase	2.5	1960	12		Tulip <i>et al.</i> (1992)
1nnmb	Fab NC10-flu neuraminidase	2.5	1500	9		Malby <i>et al.</i> (1994)
(*) ^b	Fab BH151-flu hemagglutinin X31	2.8	1550	5		Fleury <i>et al.</i> (personal communication)
(*) ^b	Fab HC45-flu hemagglutinin X31	2.8	1850	4		Fleury <i>et al.</i> (personal communication)
1dvf	Fv D1.3-Fv E5.2	1.9	1680	10	15	Braden <i>et al.</i> (1996)
1iai	Fab 730.1.4-Fab 409.5.3	2.9	1900	6		Ban <i>et al.</i> (1994)
1nfd	Fab H57-N15 T cell receptor	2.8	1710	8		Wang <i>et al.</i> (1998)
1kb5	Fab Désiré-1-TCR Fv domain	2.5	2340	15		Housset <i>et al.</i> (1997)
1ao7	T cell receptor-HLA-A2/peptide	2.6	1990	15		Garboczi <i>et al.</i> (1996)
D. Enzyme complexes (9)						
(*) ^b	β-Lactamase-BLIP	1.7	2560	11	31	Strynadka <i>et al.</i> (1996)
1brs	Barnase-barstar	2.0	1570	13	32	Buckle <i>et al.</i> (1994)
1dfj	RNase A-RNase inhibitor	2.5	2600	7		Kobe & Deisenhofer (1995)
1dhk	α-Amylase-bean inhibitor	1.9	3080	12	37	Bompard-Gilles <i>et al.</i> (1996)
1fss	Acetylcholinesterase-fasciculin	3.0	1970	7		Harel <i>et al.</i> (1995)
1gla	Glycerol kinase-Factor IIIIGlc	2.6	1300	4		Hurley <i>et al.</i> (1993)
1udi	Uracil-DNA glycosylase-inhibitor	2.7	2020	11		Savva & Pearl (1995)
1ydr	Protein kinase A-inhibitor	2.2	2000	14	6	Engh <i>et al.</i> (1996)
2pcc	Cytochrome peroxidase-cytochrome c	2.3	1170	1	15	Pelletier & Kraut (1992)
E. G-proteins, cell cycle, signal transduction (11)						
1tx4	Rho-Rho GAP	1.6	2280	14	50	Rittinger <i>et al.</i> (1997)
1gua	Rap1A-cRaf1	2.0	1310	12	7	Nassar <i>et al.</i> (1996)
1a2k	Ran-NFT2	2.5	1590	10		Stewart <i>et al.</i> (1998)
1efu	EFtu-EFts. <i>E. coli</i>	2.5	3660	11		Kawashima <i>et al.</i> (1996)
1aip	EFtu-EFts. <i>T. thermophilus</i>	3.0	2940	9		Wang <i>et al.</i> (1997)
1gg2	G _{iα1} -G _{iβ1} γ ₂	2.4	2360	13	10	Wall <i>et al.</i> (1995)
1got	Transducin G _{αγ} -G _{βγ}	2.0	2500	18	36	Lambright <i>et al.</i> (1996)
2trc	G _{βγ} -phosducin	2.4	4660	34	26	Gaudet <i>et al.</i> (1996)

1agr	G _{iα} -RGS4	2.8	1650	13		Tesmer <i>et al.</i> (1997)
1fin	CDK2-cyclin A	2.3	3400	17		Jeffrey <i>et al.</i> (1995)
1a0b	CheA-Che Y	2.9	1140	5		Welch <i>et al.</i> (1997)
F. Miscellaneous (12)						
1fc2	Protein A-Fc fragment	2.8	1300	2		Deisenhofer (1981)
1igc	Protein G-Fab MOPC21	2.6	1350	14		Derrick & Wigley (1994)
1ak4	Cyclophilin-HIV capsid	2.4	1170	8	3	Gamble <i>et al.</i> (1996)
1efn	Fyn SH3 domain-HIV Nef	2.5	1260	7		Lee <i>et al.</i> (1996)
1atn	Actin-DNase I	2.8	1780	8		Kabsch <i>et al.</i> (1990)
2btf	Actin-profilin	2.5	2090	11		Schutt <i>et al.</i> (1993)
1dkg	Grep E-DNA K	2.8	1980	4		Harrison <i>et al.</i> (1997)
1ebp	Erythropoietin receptor-peptide	2.8	1940	13		Livnah <i>et al.</i> (1996)
1hwg	HGH receptor-human growth hormone	2.5	4200	11		Sundström <i>et al.</i> (1996)
1seb	HLA DR1-enterotoxin B	2.7	1340	8		Jardetsky <i>et al.</i> (1994)
1tco	FKBP12-Calcineurin	2.5	2470	8		Griffith <i>et al.</i> (1995)
1ycs	p53-53BP2	2.2	1500	7	8	Gorina & Pavletich (1996)
Protease-inhibitor		Mean	1530	9.5	14.6	
		s.d.	170	2.3	4.7	
Large protease complexes		Mean	3300	15.8		
		s.d.	540	4.3		
Antibody-antigen		Mean	1680	8.5		
		s.d.	260	3.5		
Enzyme complexes		Mean	2030	8.9		
		s.d.	630	4.4		
G-proteins, signal transduction		Mean	2500	14.2		
		s.d.	1090	7.5		
Miscellaneous		Mean	1870	8.4		
		s.d.	840	3.4		
All complexes		Mean	1940	10.1	18.3	
		s.d.	760	4.8	11.1	

^a Number of interface solvent molecules in 36 X-ray structures with resolution 2.4 Å or better. Due to the small number of occurrences in other categories, the mean and standard deviation are quoted only for protease-inhibitor and for all complexes.

^b Co-ordinates are gift from authors. The files are referred to as *1 to *3.