

Table 1: The rate constant benchmark. Complexes overlapping with the validated set are highlighted in **bold**. The first entry refers to pdb code for the bound complex. I-RMSD values were calculated using C_{α} positions. †Personal communication

Complex	Type	Protein 1	PDB1	Protein 2	PDB2	k_{on} ($\text{mol}^{-1} \text{s}^{-1}$)	k_{off} (s^{-1})	DASA (\AA^2)	I-RMSD (\AA)	Ref.
1CBW_ABC:D	EI	Chymotrypsin	4CHA_ABC	BPTI	9PTL_A	1.7e5	1.8e-3	1457	0.74	(1)
1DFJ_E:I	EI	Ribonuclease A	9RSA_B	Rnase inhibitor	2BNH_A	1.66e8	9.8-6	2582	1.02	(2)
1E4K_AB:C	OR	FC fragment of human IgG 1	2DTQ_AB	Human FCGR III	1FNL_A	4.2e5	7.5e-1	1634	2.59	(3)
1E6E_A:B	ES	Adrenoxin reductase	1EIN_A	Adrenoxin	1CJE_D	4.434e3	3.8e-3	2315	1.33	(4)
1E6J_HL:P	A	Fab 13B5	1E6O_HL	HIV-1 capsid protein p24	1A43_A	3.5e5	1.2e-3	1245	1.05	(5)
1EER_A:BC	OR	Erythropoietin	1BUY_A	EPO receptor	1ERN_AB	2.1e7	7.8e-5	3347	2.44	(6)
1EMV_A:B	EI	Colicin E9 nuclease	1FSJ_B	Im9 immunity protein	1IMQ_A	9.0e7	2.2e-6	1535	1.28	(7)
1FFW_A:B	OX	Chemotaxis protein CheY	3CHY_A	Chemotaxis protein CheA	1FWP_A	3.68e2	1.14e-5	1170	1.43	(8)
1FSK_BC:A	AB	Fab - Birch pollen antigen Bet V1	1FSK_BC	Birch pollen antigen Bet V1	1BV1_A	1.0e5	2.5e-5	1623	0.45	†
1GLL_A:I	EI	Chymotrypsin	4CHA_ABC	PMP-C (LCMI II)	1PMC_A(6)	8.00e5	1.62e-4	1595	1.2	(9)
1GXD_A:C	EI	ProMMP2 type IV collagenase	1CK7_A	Metalloproteinase inhibitor 2	1BR9_A	1.4e5	7e-4	2445	1.39	(10)
1J1W_P:I	EI	Alkaline metallo-proteinase	1AKL_A	Proteinase inhibitor	2RN4_A(1)	2.5e5	1.15e-6	2018	2.07	(11)
1JMO_A:HL	ER	Heparin cofactor	1JMJ_A	Thrombin	2CN0_HL	2.23e2	2.5e-5	3461	3.21	(12)
1JPS_HL:T	A	Fab D3H44	1JPT_HL	Tissue factor	1TFH_B	9.8e5	1e-4	1852	0.51	(13)
1JTG_B:A	EI	β -lactamase inhibitor protein	3GMU_B	β -lactamase TEM-1	1ZG4_A	3.1e5	1.2e-4	2600	0.49	(14)
1JWH_CD:A	ER	Casein kinase II β chain	3EED_AB	Casein kinase II α chain	3C13_A	6.65e4	3.6e-4	1451	1.27	(15)
1KAC_A:B	OR	Adenovirus fiber knob protein	1NOB_F	Adenovirus receptor	1F5W_B	1.8e5	2.8e-3	1456	0.95	(16)
1KKL_ABC:H	ES	HPr kinase C-ter domain	1JB1_ABC	HPr	2HPR_A	1.3e5	5.8e-3	1641	2.2	(17)
1KLU_AB:D	OX	MHC class 2 HLA-DR1	1H15_AB	Staphylococcus enterotoxin C3	1STE_A	5.22e3	2.4e-2	1254	0.43	(18)
1KTZ_A:B	OR	TGF- β	1TGG_A	TGF- β receptor	1M9Z_A	7.4e5	5.4e-2	989	0.39	(19)
1KXQ_H:A	AB	Camel VHH - Pancreatic α -amylase	1KXQ_H	Pancreatic α -amylase	1PPL_A	2.36e5	8e-4	2172	0.72	(20)
1LFD_B:A	OG	Ras.GNP	5P21_A	RalGDS Ras-interacting domain	1LXD_A	7.7e6	1.49e1	1167	1.79	(21)
1MAH_A:F	EI	Acetylcholinesterase	1J06_B	Fasciculin	1FSC_A	2.7e7	2.9e-5	2145	0.61	(22)
1MLC_AB:E	A	Fab44.1	1MLB_AB	HEW lysozyme	3LZT_A	1e4	9.1e-4	1392	0.6	(23)
1MQ8_A:B	OX	ICAM-1 domain 1-2	1IAM_A	Integrin α -L I domain	1MQ9_A	1.33e5	4.3e-1	1241	1.76	(24)
1P2C_AB:C	A	FabF10.6.6	2Q76_AB	HEW lysozyme	3LZT_A	4.21e4	2.92e-3	1456	0.46	(25)
1PPE_E:I	EI	Trypsinogen	2PTN_A	CMTI-1 squash inhibitor	1LU0_A	6.7e6	2.5e-5	1688	0.34	(26)
1T6B_X:Y	OR	Anthrax protective antigen	1ACC_A	Anthrax toxin receptor	1SHU_X	5.3e4	9.2e-6	1948	0.62	(27)
1VFB_AB:C	A	Fv D1.3	1VFA_AB	HEW lysozyme	8LYZ_A	1.39e6	5.14e-3	1383	1.02	(28)
1XUL_ABD:T	OR	TNF domain of APRIL	1U5Y_ABD	TACI CRD2 domain	1XUT_A(11)	9.22e5	5.89e-3	1700	1.3	(29)
2AJF_A:E	OR	Angiotensin-converting enzyme 2	1R42_A	SARS spike protein receptor binding domain	2GHV_E	7.12e4	1.16e-3	1704	0.65	(30)
2B42_A:B	EI	Xylanase	2DCY_A	Xylanase inhibitor	1T6E_X	3.61e5	3.6e-4	2520	0.72	(31)
2B4L_AB:C	OX	Integrase (HIV-1)	1BIZ_AB	PC4 and SFRS1 interacting protein	1Z9E_A(1)	4.75e5	3.9e-3	1259	0.99	(32)
2GOX_A:B	OX	Complement C3d fragment	1C3D_A	Staphylococcus aureus Efb-C	2GOM_A	4.04e5	5.63e-4	1631	0.6	(33)
2I25_N:L	A	Shark single domain antigen receptor	2I24_N	HEW lysozyme	3LZT_A	9e4	1e-4	1425	1.21	(34)
2I9B_E:A	OR	uPAR surface receptor	1YWH_A	Urokinase-type plasminogen activator	2I9A_A	1.19e5	1.14e-4	2382	3.79	(35)
2OZA_B:A	OX	MAP kinase 14	3HEC_A	MAP kinase-activated protein kinase 2	3FYK_X	8.1e7	8e-2	6254	1.89	(36)
2PTC_E:I	EI	Trypsinogen	2PTN_A	BPTI	9PTL_A	1.1e6	6.6e-8	1429	0.28	(37)
2SIC_E:I	EI	Subtilisin	1SUP_A	Streptomyces subtilisin inhibitor	3SSL_A	6.5e6	9e-5	1617	0.36	(38)
2SNI_E:I	EI	Subtilisin	1UBN_A	Chymotrypsin inhibitor 2	2CI2_I	3.1e6	6.1e-6	1628	0.35	(39)
2VIR_AB:C	A	Fab	1GIG_LH	Flu virus hemagglutinin	2HMG_AB	1.1e5	1.1e-4	1263	0.8	(40)
2VIS_AB:C	A	Fab	1GIG_LH	Flu virus hemagglutinin	2VIU_ACE	5.4e2	2.16e-3	1296	0.8	(40)
2WPT_A:B	EI	Colicin E9 nuclease	1FSJ_B	Im2 immunity protein	2NO8_A	5e7	7.3e-1	1581	1.61	(41)
3BP8_AB:C	OX	Mlc transcription regulator	1Z6R_AB	PTS glucose-specific enzyme EIICB	3BP3_A	9.95e5	3.85e-3	1398	0.45	(42)

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