

TableS1. Complete Benchmark 4.0

Complex	Cat.	PDB ID 1	Protein 1	PDB ID 2	Protein 2	I-RMSD (Å)	Δ ASA(Å ²)	BM version ^a
Rigid-body (121)								
1AHW_AB:C	A	1FGN_LH	Fab 5g9	1TFH_A	Tissue factor	0.69	1899	2
1BVK_DE:F	A	1BVL_BA	Fv Hulys11	3LZT_	HEW lysozyme	1.24	1321	2
1DQJ_AB:C	A	1DQQ_CD	Fab Hyhel63	3LZT_	HEW lysozyme	0.75	1765	2
1E6J_HL:P	A	1E6O_HL	Fab	1A43_	HIV-1 capsid protein p24	1.05	1245	2
1JPS_HL:T	A	1JPT_HL	Fab D3H44	1TFH_B	Tissue factor	0.51	1852	2
1MLC_AB:E	A	1MLB_AB	Fab44.1	3LZT_	HEW lysozyme	0.6	1392	2
1VFB_AB:C	A	1VFA_AB	Fv D1.3	8LYZ_	HEW lysozyme	1.02	1383	2
1WEJ_HL:F	A	1QBL_HL	Fab E8	1HRC_	Cytochrome C	0.31	1177	2
2FD6_HL:U	A	2FAT_HL	Plasminogen receptor antibody	1YWH_A	Plasminogen activator receptor	1.07	1139	3
2I25_N:L	A	2I24_N	Shark single domain antigen receptor	3LZT	Lysozyme	1.21	1425	3
2VIS_AB:C	A	1GIG_LH	Fab	2VIU_ ACE	Flu virus hemagglutinin	0.8	1296	2
1BJ1_HL:VW	AB	1BJ1_HL	Fab	2VPF_GH	VEGF	0.5	1731	2
1FSK_BC:A	AB	1FSK_BC	Fab	1BV1_	Birch pollen antigen Bet V1	0.45	1623	2
1I9R_HL:ABC	AB	1I9R_HL	Fab	1ALY_ABC	Cd40 ligand	1.3	1498	2
1IQD_AB:C	AB	1IQD_AB	Fab	1D7P_M	Factor VIII domain C2	0.48	1976	2
1K4C_AB:C	AB	1K4C_AB	Fab	1JVM_ABCD	Potassium Channel Kcsa	0.53	1601	2
1KXQ_H:A	AB	1KXQ_H	Camel VHH	1PPI_	Pancreatic alpha-amylase	0.72	2172	2
1NCA_HL:N	AB	1NCA_HL	Fab	7NN9_	Flu virus neuraminidase N9	0.24	1953	2
1NSN_HL:S	AB	1NSN_HL	Fab N10	1KDC_	Staphylococcal nuclease	0.35	1776	2
1QFW_HL:AB	AB	1QFW_HL	Fv	1HRP_AB	Human chorionic gonadotropin	1.31	1580	2
1QFW_IM:AB	AB	1QFW_IM	Fv	1HRP_AB	Human chorionic gonadotropin	0.73	1637	2
2JEL_HL:P	AB	2JEL_HL	Fab Jel42	1POH_	HPr	0.17	1501	2
1AVX_A:B	E	1QQU_A	Porcine trypsin	1BA7_B	Soybean trypsin inhibitor	0.47	1585	2
1AY7_A:B	E	1RGH_B	Barnase	1A19_B	Barstar	0.54	1237	2
1BVN_P:T	E	1PIG_	α -amylase	1HOE_	Tendamistat	0.87	2222	2
1CGI_E:I	E	2CGA_B	Bovine chymotrypsinogen	1HPT_	PSTI	2.02	2053	2
1CLV_A:I	E	1JAE_A	α -amylase	1QFD_A(1)	α -amylase inhibitor	0.86	2087	4
1D6R_A:I	E	2TGT_	Bovine trypsin	1K9B_A	Bowman-Birk inhibitor	1.14	1408	2
1DFJ_E:I	E	9RSA_B	Ribonuclease A	2BNH_	Rnase inhibitor	1.02	2582	2
1E6E_A:B	E	1E1N_A	Adrenoxin reductase	1CJE_D	Adrenoxin	1.33	2315	2

1EAW_A:B	E	1EAX_A	Matriptase	9PTI_	BPTI	0.54	1866	2
1EWY_A:C	E	1GJR_A	Ferredoxin reductase	1CZP_A	Ferredoxin	0.8	1502	2
1EZU_C:AB *	E	1TRM_A	D102N Trypsin	1ECZ_AB	Ecotin	1.21	2751	2
1F34_A:B	E	4PEP_	Porcine pepsin	1F32_A	Ascaris inhibitor 3	0.93	3038	2
1FLE_E:I	E	9EST_A	Elastase	2REL_A(4)	Elafin	1.02	1763	4
1GL1_A:I	E	1K2I_1	α -chymotrypsin	1PMC_A(6)	Protease inhibitor LCMI II	1.21	1591	4
1GXD_A:C	E	1CK7_A	proMMP2 type IV collagenase	1BR9_A	Metalloproteinase inhibitor 2	1.39	2445	4
1HTA_AB:I	E	2PKA_XY	Kallikrein	1BX8_	Hirustatin	1.4	1737	2
1JTG_B:A	E	3GMU_B	β -lactamase inhibitor protein	1ZG4_A	β -lactamase TEM-1	0.49	2600	4
1MAH_A:F	E	1J06_B	Acetylcholinesterase	1FSC_	Fasciculin	0.61	2145	2
1N80_ABC:E *	E	8GCH_A	Chymotrypsin	1IFG_A	Ecotin	0.94	1851	3
1OC0_A:B	E	1B3K_A	Plasminogen activator inhibitor-1	2JQ8_A(4)	Vitronectin Somatomedin B domain	1	1313	4
1OPH_A:B	E	1Q1P_A	α -1-antitrypsin	1UTQ_A	Trypsinogen	1.21	1360	3
1OYV_B:I	E	1SCD_A	Subtilisin Carlsberg	1PJU_A	Two-headed tomato inhibitor-II	0.5	1280	4
1OYV_A:I	E	1SCD_A	Subtilisin Carlsberg	1PJU_A	Two-headed tomato inhibitor-II	0.7	1930	4
1PPE_E:I	E	1BTP_	Bovine trypsin	1LU0_A	CMTI-1 squash inhibitor	0.44	1688	2
1ROR_E:I	E	1SCN_E	Subtilisin carlsberg	2GKR_I	OMTKY	0.45	1409	3
1TMQ_A:B	E	1JAE_	alpha-amylase	1B1U_A	RAGI inhibitor	0.86	2401	2
1UDI_E:I	E	1UDH_	Uracyl-DNA glycosylase	2UGI_B	Glycosylase inhibitor	0.9	2022	2
1YVB_A:I	E	2GHU_A	Falcipain 2	1CEW_I	Cystatin	0.51	1743	3
2ABZ_B:E	E	3I1U_A	Carboxypeptidase A1	1ZFI_A(1)	Leech carboxypeptidase inhibitor	0.9	1443	4
2B42_A:B	E	2DCY_A	Xylanase	1T6E_X	Xylanase inhibitor	0.72	2520	3
2J0T_A:D	E	966C_A	MMP1 Intersitial collagenase	1D2B_A(20)	Metalloproteinase inhibitor 1	1.23	1477	4
2MTA_HL:A	E	2BBK_JM	Methylamine dehydrogenase	2RAC_A	Amicyanin	0.41	1461	2
2O8V_A:B	E	1SUR_	PAPS reductase	2TRX_A	Thioredoxin	1.37	1619	3
2OUL_A:B	E	3BPF_A	Falcipain 2	2NNR_A	Chagasin	0.53	1933	4
2PCC_A:B	E	1CCP_	Cyt C peroxidase	1YCC_	Cytochrome C	0.39	1141	2
2SIC_E:I	E	1SUP_	Subtilisin	3SSI_	Streptomyces subtilisin inhibitor	0.36	1617	2
2SNI_E:I	E	1UBN_A	Subtilisin	2CI2_I	Chymotrypsin inhibitor 2	0.35	1628	2
2UUY_A:B	E	1HJ9_A	Trypsin	2UUX_A	Tryptase inhibitor from tick	0.43	1280	3

3SGQ_E:I	E	2QA9_E	Streptogrisin B	2OVO_A	Ovomucoid inhibitor third domain	0.39	1211	4
7CEI_A:B	E	1UNK_D	Colicin E7 nuclease	1M08_B	Im7 immunity protein	0.7	1384	2
1A2K_C:AB	O	1QG4_A	Ran GTPase	1OUN_AB	Nuclear transport factor 2	1.11	1603	2
1AK4_A:D	O	2CPL_	Cyclophilin	1E6J_P	HIV capsid	1.33	1029	2
1AKJ_AB:DE	O	2CLR_DE	MHC class 1 HLA-A2	1CD8_AB	T-cell CD8 coreceptor	1.14	1995	2
1AZS_AB:C	O	1AB8_AB	Adenylyl cyclase	1AZT_A	AC activator Gs α complex	0.72	1911	3
1B6C_A:B	O	1D6O_A	FKBP binding protein	1IAS_A	TGFbeta receptor	1.96	1752	2
1BUH_A:B	O	1HCL_	CDK2 kinase	1DKS_A	Ckshs1	0.75	1324	2
1E96_A:B	O	1MH1_	Rac GTPase	1HH8_A	p67 Phox	0.71	1179	2
1EFN_B:A	O	1AVV_A	HIV-1-NEF protein	1G83_A	SH3 domain	0.77	1254	3
1F51_AB:E	O	1IXM_AB	Sporulation response factor B	1SRR_C	Sporulation response factor F	0.74	2407	2
1FC2_C:D	O	1BDD_	Staphylococcus Protein A	1FC1_AB	Human Fc fragment	1.69	1307	2
1FCC_AB:C	O	1FC1_AB	Fc domain of IgG1 MO61	2IGG_A(3)	Strep. protein G C2 fragment	0.93	1354	4
1FFW_A:B	O	3CHY_A	Chemotaxis protein CheY	1FWP_A	Chemotaxis protein CheA	1.43	1166	4
1FQJ_A:B	O	1TND_C	Gt-alpha	1FQI_A	RGS9	0.91	1806	2
1GCQ_B:C	O	1GRI_B	GRB2 C-ter SH3 domain	1GCP_B	GRB2 N-ter SH3 domain	0.92	1208	2
1GHQ_A:B	O	1C3D_	Complement C3	1LY2_A	Epstein-Barr virus receptor CR2	0.34	800	2
1GLA_G:F	O	1BU6_0	Glycerol Kinase	1F3Z_A	Glucose specific phosphocarrier	0.98	1304	3
1GPW_A:B	O	1THF_D	HISF protein	1K9V_F	Amidotransferase HISH	0.65	2097	3
1H9D_A:B	O	1EAN_A	Runx1 domain of CBF α 1	1ILF_A(1)	Dimerisation domain of CBF- β	1.32	2121	4
1HCF_AB:X	O	1B98_AM	Neurotrophin-4	1WWB_X	TrkB-d5 growth factor receptor	0.88	2136	4
1HE1_C:A	O	1MH1_	Rac GTPase	1HE9_A	Pseudomonas toxin GAP dom.	0.93	2113	2
1I4D_D:AB	O	1MH1_	Rac GTPase	1I49_AB	Arfaptin	1.41	1657	2
1J2J_A:B	O	1O3Y_A	Arf1 GTPase	1OXZ_A	GAT domain of GGA1	0.63	1209	3
1JWH_CD:A	O	3EED_AB	Casein kinase II β chain	3C13_A	Casein kinase II α chain	1.27	1452	4
1K74_AB:DE	O	1MZN_AB	RXR- α	1ZGY_AB	PPAR-gamma	0.8	2200	3
1KAC_A:B	O	1NOB_F	Adenovirus fiber knob protein	1F5W_B	Adenovirus receptor	0.95	1456	2
1KLU_AB:D	O	1H15_AB	MHC class 2 HLA-DR1	1STE_	Staphylococcus enterotoxin C3	0.43	1254	2
1KTZ_A:B	O	1TGK_	TGF- β	1M9Z_A	TGF- β receptor	0.39	989	2
1KXP_A:D	O	1IJJ_B	Actin	1KW2_B	Vitamin D binding protein	1.12	3341	2

1ML0_AB:D	O	1MKF_AB	Viral chemokine binding p. M3	1DOL_	Chemokine Mcp1	1.02	2069	2
1OFU_XY:A	O	1OFT_AB	SulA (PA3008)	2VAW_A	Cell division protein FtsZ	1.1	1583	4
1PVH_A:B	O	1BQU_A	IL6 receptor β chain D2-D3 domains	1EMR_A	Leukemia inhibitory factor	0.34	1403	4
1QA9_A:B	O	1HNF_	CD2	1CCZ_A	CD58	0.73	1353	2
1RLB_ABCD:E	O	2PAB_ABCD	Transthyretin	1HBP_	Retinol binding protein	0.66	1439	2
1RV6_VW:X	O	1FZV_AB	PIGF receptor binding domain	1QSZ_A	Flt1 protein domain 2	1.09	1626	4
1S1Q_A:B	O	2F0R_A	UEV domain	1YJ1_A	Ubiquitin	0.98	1288	3
1SBB_A:B	O	1BEC_	T-cell receptor β	1SE4_	Staphylococcus enterotoxin B	0.37	1064	2
1T6B_X:Y	O	1ACC_	Anthrax protective antigen	1SHU_X	Anthrax toxin receptor	0.62	1948	3
1US7_A:B	O	2FXS_A	Heat shock protein 82 N-ter domain	2W0G_A	HSP 90 co-chaperone CDC37 C-ter domain	1.06	1095	4
1WDW_BD:A	O	1V8Z_AB	Tryptophan synthase β chain 1	1GEQ_A	Tryptophan synthase α chain	1.29	3148	4
1XD3_A:B	O	1UCH	UCH-L3	1YJ1_A	Ubiquitin	1.24	2281	3
1XU1_ABD:T	O	1U5Y_ABD	TNF domain of APRIL	1XUT_A(11)	TNF receptor superfamily member 13B TACI CRD2 domain	1.3	1697	4
1Z0K_A:B	O	2BME_A	Rab4A GTPase	1YZM_A	RAB4 binding domain of Rabenosyn	0.53	1787	3
1Z5Y_D:E	O	1L6P	N-term of DsbD	2B1K_A	E.coli CCMG protein	1.23	1346	3
1ZHH_A:B	O	1JX6_A	Autoinducer 2-binding periplasmic protein LuxP	2HJE_A	Autoinducer 2 sensor kinase/phosphatase LuxQ	1.31	2189	4
1ZHI_A:B	O	1M4Z_A	BAH domain of Orc1	1Z1A_A	Sir Orc-interaction domain	0.68	1322	3
2A5T_A:B	O	1Y20_A	NMDA receptor R1-4A subunit ligand-binding core	2A5S_A	NMDA receptor R2A subunit ligand-binding core	1.28	1892	4
2A9K_A:B	O	1u90_A	Ras-related protein Ral-A	2C8B_X	Mono-ADP-ribosyltransferase C3	0.85	1751	4
2AJF_A:E	O	1R42_A	ACE2	2GHV_E	SARS spike protein receptor binding domain	0.65	1704	3
2B4J_AB:C	O	1BIZ_AB	Integrase (HIV-1)	1Z9E_A(1)	PC4 and SFRS1 interacting protein	0.99	1273	4
2BTF_A:P	O	1IJJ_B	Actin	1PNE_	Profilin	0.75	2063	2
2FJU_B:A	O	2ZKM_X	Phospholipase β 2	1MH1_A	Rac GTPase	1.04	1245	4
2G77_A:B	O	1FKM_A	GTPase-activating protein GYP1	1Z06_A	Ras-related protein Rab-33B	1.75	2524	4
2HLE_A:B	O	2BBA_A	Ephrin B4 receptor	1IKO_P	Ephrin B2 ectodomain	1.4	2116	3
2HQ5_A:H	O	1CRZ_A	TolB	1OAP_A	Pal	1.14	2333	3

2O0B_A:B	O	2O0A_A	Ubiquitin ligase	1YJ1_A	Ubiquitin	0.85	808	3	
2O0R_AB:C	O	1L7E_AB	NAD(P) transhydrogenase subunit α part 1	1E3T_A	NAD(P) transhydrogenase subunit beta	1.42	2065	4	
2VDB_A:B	O	3CX9_A	Serum albumin	2J5Y_A	Peptostreptococcal albumin-binding protein	0.47	1798	4	
3BP8_AB:C	O	1Z6R_AB	Mlc transcription regulator	3BP3_A	PTS glucose-specific enzyme EIICB	0.45	1391	4	
3D5S_A:C	O	1C3D_A	Complement C3d fragment	2GOM_A	Fibrinogen-binding protein C-ter domain	0.56	1620	4	
Medium Dfficulty (30)									
1BGX_HL:T	A	1AY1_HL	Fab	1CMW_A	Taq polymerase	1.48	5814	2	
1ACB_E:I	E	2CGA_B	Chymotrypsin	1EGL_	Eglin C	2.26	1544	2	
1IJK_A:BC	E	1AUQ_	Von Willebrand Factor dom. A1	1FVU_AB	Botrocetin	0.68	1648	2	
1JIW_P:I	E	1AKL_A	Alkaline metalloproteinase	2RN4_A(1)	Proteinase inhibitor	2.07	1997	4	
1KKL_ABC:H	E	1JB1_ABC	HPr kinase C-ter domain	2HPR_	HPr	2.2	1641	2	
1M10_A:B	E	1AUQ_	Von willebrand factor dom. A1	1M0Z_B	Glycoprotein IB- α	2.1	2097	2	
1NW9_B:A	E	1JXQ_A	Capase-9	1IFG_A	Ecotin	1.97	2112	3	
4CPA_A:I	E	8CPA_A	Carboxypeptidase A	1H20_A(9)	Potato carboxypeptidase inhibitor	1.97	1175	4	
1GP2_A:BG	O	1GIA_	Gi- α	1TBG_DH	Gi- β, γ	1.65	2287	2	
1GRN_A:B	*	O	1A4R_A	CDC42 GTPase	1RGP_	CDC42 GAP	1.22	2332	2
1HE8_B:A	O	821P_	Ras GTPase	1E8Z_A	PIP3 kinase	0.92	1305	2	
1I2M_A:B	O	1QG4_A	Ran GTPase	1A12_A	RCC1	2.12	2779	2	
1IB1_AB:E	O	1QJB_AB	14-3-3 protein	1KUY_A	Serotonin N-acteylase	2.09	2808	2	
1K5D_AB:C	O	1RRP_AB	Ran GTPase	1YRG_B	Ran GAP	1.19	2527	2	
1LFD_B:A	O	5P21_A	Ras	1LXD_A	RalGDS Ras-interacting domain	1.79	1167	4	
1MQ8_A:B	O	1IAM_A	ICAM-1 domain 1-2	1MQ9_A	Integrin α -L I domain	1.76	1253	4	
1N2C_ABCD:EF	O	3MIN_ABCD	Nitrogenase Mo-Fe protein	2NIP_AB	Nitrogenase Fe protein	2.13	3635	2	
1R6Q_A:C	O	1R6C_X	Clp protease subunit ClpA	2W9R_A	Clp protease adaptor protein ClpS	1.67	1651	4	
1SYX_A:B	O	1QGV_A	Spliceosomal U5 15 kDa protein	1L2Z_A(1)	CD2 receptor binding protein 2 C-ter fragment	1.64	1293	4	
1WQ1_R:G	*	O	6Q21_D	Ras GTPase	1WER_	Ras GAP	1.16	2913	2
1XQS_A:C	O	1XQR_A	HspBP1	1S3X_A	Hsp70 ATPase domain	1.77	2350	3	
2AYO_A:B	O	2AYN_A	Ubiquitin carboxyl-terminal hydrolase 14	2FCN_A	Ubiquitin	1.62	3027	4	
2CFH_A:C	O	1S27_A	BET3	2BJN_A	TPC6	1.55	2384	3	

2H7V_A:C	O	1MH1_	Rac GTPase	2H7O_A	YpkA	1.63	1574	3
2HRK_A:B	O	2HRA_A	Glutamyl-t-RNA synthetase	2HQT_A	GU-4 nucleic binding protein	2.03	1595	3
2J7P_A:D	O	1NG1_A	SRP GTPase Ffh	2IYL_D	Cell division protein FtsY	1.93	3008	4
2NZ8_A:B	O	1MH1_	Rac GTPase	1NTY_A	DH/PH domain of TRIO	2.13	2599	3
2OZA_B:A	O	3HEC_A	MAP kinase 14	3FYK_X	MAP kinase-activated protein kinase 2	1.89	6248	4
2Z0E_A:B	O	2D1I_A	Cysteine protease Atg4B	1V49_A(1)	Microtubule-associated proteins 1A/1B light chain 3B	2.15	2478	4
3CPH_G:A	O	3CPI_G	Ras-related protein Sec4	1G16_A	Rab GDP-dissociation inhibitor	2.12	1685	4
Difficult (25)								
1E4K_AB:C	A	2DTQ_AB	FC fragment of human IgG 1	1FNL_A	Human FCGR III	2.59	1634	3
2HMI_CD:AB	AB	2HMI_CD	Fab 28	1S6P_AB	HIV1 reverse transcriptase	2.26	1234	2
1F6M_A:C	E	1CL0_A	Thioredoxin reductase	2TIR_A	Thioredoxin 1	4.9	1821	4
1FQ1_A:B	E	1B39_A	CDK2 kinase	1FPZ_F	CDK inhibitor 3	3.41	1832	2
1PXV_A:C	E	1X9Y_A	Cystein protease	1NYC_A	Cystein protease inhibitor	2.63	2336	3
1ZLI_A:B	E	1KWM_A	Carboxypeptidase B	2JTO_A(6)	Tick carboxypeptidase inhibitor	2.53	2084	4
2O3B_A:B	E	1ZM8_A	NucA nuclease	1J57_A	NuiA nuclease inhibitor	3.13	1675	4
1ATN_A:D	O	1IJJ_B	Actin	3DNI_	Dnase I	3.28	1774	2
1BKD_R:S	O	1CTQ_A	Ras GTPase	2IIO_B	Son of sevenless	2.86	3163	3
1DE4_AB:CF	O	1A6Z_AB	β 2-microglobulin	1CX8_AB	Transferrin receptor ectodom.	2.59	2066	2
1EER_A:BC	O	1BUY_A	Erythropoietin	1ERN_AB	EPO receptor	2.44	3347	2
1FAK_HL:T	O	1QFK_HL	Coagulation factor VIIa	1TFH_B	Soluble tissue factor	6.18	3363	2
1H1V_A:G	O	1IJJ_B	Actin	1D0N_B	Gelsolin	6.62	2071	2
1IBR_A:B	O	1QG4_A	Ran GTPase	1F59_A	Importin beta	2.54	2270	2
1IRA_Y:X	O	1G0Y_R	Interleukin-1 receptor	1ILR_1	Interleukin-1 receptor antagonist protein	8.38	3367	3
1JK9_B:A	O	1QUP_A	CCS metallochaperone	2JCW_A	SOD1 superoxide dismutase	4.87	2130	4
1JMO_A:HL	O	1JMJ_A	Heparin cofactor	2CN0_HL	Thrombin	3.21	3461	3
1JZD_AB:C	O	1JZO_AB	DsbC disulfide bond isomerase	1JPE_A	DsbD disulfide bond isomerase	2.71	2026	4
1R8S_A:E	O	1HUR_A	Arf1 GTPase	1R8M_E	Sec 7 domain	3.73	2986	3
1Y64_A:B	O	2FXU_A	Actin	1UX5_A	BN11 protein	4.69	2745	3
1ZM4_A:B	O	1NOV_C	Elongation factor 2	1XK9_A	Diphtheria toxin A catalytic domain	2.94	1554	4
2COL_A:B	O	1FCH_A	PTS1 and TRP region of PEX5	1C44_A	SCP2	2.62	2013	3

2I9B_E:A	○	1YWH_A	Urokinase plasminogen activator surface receptor	2I9A_A	Urokinase-type plasminogen activator	3.79	2371	4
2IDO_A:B	○	1J54_A	DNA polymerase III ϵ exonuclease domain	1SE7_A(1)	HOT protein (P1 phage)	2.79	1953	4
2OT3_B:A	○	1YZU_A	Rab21 GTPase	1TXU_A	Rabex-5 VPS9 domain	2.79	2306	3

^a Benchmark version that the case was/is included.