

1CRLJA	109	kag.....A..NL.....P..VMLWIFGGfevG...GTs.....T.....Pp..Aq.Mitksia.....Mgkp.....IIH...VS.....	153
2ES4JA	7T..R.....Y..PVLLVHGLA...G...TD.....K.....A...N...Vvdywygigsdlq...Shgakv...YVA...NL.....	49
3H2GJA	59E.....PatasGVLLTGG...GercSGpypll.....GghptealrageqakeirdakgddplV...Tr..La...Sgg...YVV...VG.....	122
3QITJA	25E..H.....P..VVLCTHGIL..E..QGL.....Aqev...Al..Pl.Aa...Qg...YRV...VA.....	58
3C5WJP	41E..G.....P..VLLLLHGCG..H..SAL.....Savf...T...Aa..Ii...Srvq...CRI...VA.....	75
2PL5JA	44S..Kn.....N..AIIICHALS...G...Dhaaagyhsqsdkpgwddy...IggpgKs.Fdt...Nq...YFI...TC.....	94
3BF8JA	15N..N.....S..PIVIVHGLF...G...SLd...NLgvl...A...Rd..Lw...Nd...HNT...IQ.....	47
2Y6UJA	51T..R.....L..NLVFFHGSG...M...SKv...Veyy...L...Pr..Lvaa...Daegn...YADkvlL...91	91
2D5LJA	481	pa.....K..Ky.....P..VIVVYVGGP...H..AQLvtk...Trrsvvggw...D...Iy..Ma...Qkg...YAV...FT.....	524
2VTVJA	39T..K.....T..PVIFVHGNG...D..NAI...Sdmp...P..Gn..VsgygtparsvyaekArgyndceiFGVty..LsSseq	98
4G5XJA	23E..G.....A..PLLMTHGNS...S..SGA...Ilapq...L...EgeIg...Kh...WRV...LA.....	56
3DDUJA	428	gidasyqvtvqifypskdGtkipmfivhkkkikldgshP...AFIYVGG...GfniSItP...Nys...Vsr..LifV...Rhmggi...LAV...--500	500
4QPMJA	43T..K.....P..TLLLVHGLA...G...SRD...Nnrsv...A...Hy..Lt...Tn...YHV...LI.....	75
2QM0JA	32K..Pkr.....P..AIFTYHDVG...L..NYkscfqplf...Rgd...M...Qe..Ii...Qn...FVR...VH.....	72
1HLGJA	49Q..R.....P..VVFLVHGLL...A...SAT...Nisnlpnns...L...Afila...Dag...YDV...WL.....	88
1LPAJB	68N..R.....K..TRFIDHGFI...D..KGe...Nlanv...C...Kn..Lfkv...Es...VNC...TC.....	104
1AZWJA	33H..G.....K..PVVMLHGCP...G...GGcndkmr...R...H...D..P...Ak...YRT...VL.....	65
3AZPJA	422E..Lp.....P..YVVMHGGSP...T..SRvpa...VLldd...V...Ay..Ft...Srg...IGV...AD.....	458
position		10 20 30	
1CRLJA	154	.VNYRVSS...Wcfl..AGdeikaegsan.....AGLk.....DQrL.G...MqwaDNiaafgg.DP.T.K.V.T.IFGSAGS-M.....SVMChllwndgdN..T..YKg..KplERA...GIM...O	240
2ES4JA	50	-SGF.QsddgpN...--V.KQVlaat..GA.T.K.V.N.LIGHGOGGLT...SRYV..A...A.VA..PQ...L..VAS...VTM...I	110
3H2GJA	123	SDYL.G...Lc...Ksnyahpylh...SAsasati..DA.MrAars..V..I.QHk...TP.LsgK..V.M.LSGVSGGHT...AMAT.Q...R..EI...Ea..H..LSKefhLVAI	205
3QITJA	59	FDLF.G...Hc...RSshlemvtsyslt...FLA...Q..D.R..V..I.QEL...PD.Q.P.L.L.LVCHSMGAML...ATAI..A...S.VR..FK..K..LIL..V	126
3C5WJP	76	DLR.S...Hc...ETkvknpedlsaet...MAK...D.V.G.N...V..V.EAMygd..LP.P.P..I.M.LICHAMGAL...AVHT..A...S..SNlvP...LLG...LCM...I	146
2PL5JA	95	SNVI.Ggc...KssgpLSihpetstpygsrpfv...SIQ...D.M.V.Kaql..E..V.ESE...GI.E.K..L.FcVAGSMGEMQ...ALEW.S...I..AY..PN...S..LSN...CTV...M	176
3BF8JA	48	VDVR.N...Hc...LSprepvmnypa...MAO...D..V.D...T..L.DAQ...QI.D.K..A.T.FICHSMGKA...VMAL.T...A..LA..PD...R..IDK...LVA...I	112
2Y6UJA	92	IDQV.N...Hc...DSavnrrgrlgtfnwid...GAR...D.V.L.KiatxeIgs..D...S.HpaLnV.VICHSMGEGFO...ALADv...L..Q...PN...L..FHL...LIL...I	600
2D5LJA	525	VDSP...G...SAnrgaafeqvihrrlgt...EMA...D.Q.M.C...G..V.DFKsqswvDA.D.R..I.G.VHGMVSYGFM...TTNL.M...L..TH..GD...V..FKV...GVA...G	168
2VTVJA	99	gsAQY.N...YH...SS...TKY...A.I.Kt...F..I.DKVkayt..GK.S.Q..V.D.IVHSMGVSM...SLAT.L...QyyNN..WT...S..VRK...FIN...L	161
4G5XJA	57	FDLP.G...Hc...KStdaidpdrsystemeg...YAD...AM.T.E...V..M.QQL...GI.A.D..A.V.VFGMLGSHI...GIEM.I...A..RY..PE...-MRG...LMI...T	124
3DDUJA	501	ANIRGGge...Yc...ETwhkkggilankqn...CFD...DF.Q.Caaey..L..I.KEGyt...SP.K.R..L.T.INGGNGGLLva...A-C.A...N..QR..PD...L..EGC...VIA...Q	576
4QPMJA	76	FDLP.G...Sc...ETivsqdfdyvsn...LAE...KL.R.R...F..V.EAA...NL.Kgp..I.H.LACHSLGSI...ALLY..A...G..QY..PF..E..TKS...LFL..V	143
2QM0JA	73	VDAP.Gme...Ec...APvfpIgyqyp...SLD...Q..A.Dmipc..I..L.QY...NF.S.T..I.I.GVGVGACAYI...LSRY..A...L..NH..PD...T..VEG...LVL...I	142
1HLGJA	89	GNSR.G...NT...WarrnlypsdsvefwafsfdemAKY...D..P..Atidf..I..V.KKT...GQ.K.Q..L.H.YVCHGOGTLI...GFIA.F...S..TN..PslakR..TKT...FYA...L	171
1LPAJB	105	VDWK...Gcs...RTgytq...ASQnirivagV..A.Y...E.FLqsafgySP.S.N..V.H.VICHSLGHA...AGEA.G...R..RT..NG...T..IGR...ITG...L	176
1AZWJA	66	FDQR.G...Sc...RStphadlvdnntwd...LVA...D..E.R...L..R.THL...GV.D.R..W.Q.VFGGSGWSTL...ALAY..A...Q..TH..PQ...Q..VTE...LVL...R	133
3AZPJA	459	VNYG...G...Tgygrayrerlrgrwgvv...DVE...D.C.A.A...V..A.TAlaegtADR.A.R..L.A.VRCGAAGWTaasslvst...D...V..YAC...GTV...L	533
position		40 50 60 70 80	
1CRLJA	325Egk..Ya...NI.....E...VIL-G.....DQNDegtffgtsslN.....VTTDAqareyfkqs	365
2ES4JA	212	taiqptstvlgv...T...G...AT.....DtsstgldvanvtdpstlallatgaVMNrasgqndglvrcsslfgqvistsywhnhldeinqllgvrGANaedpvavirthvn.....RLKLQ	317
3H2GJA	316Rnn..LlewapQT...P...TLICG...SSNDa...T...PLK...234	342
3QITJA	229S...L...QV...TTLVY...G...DSSklnrpe...248	248
3C5WJP	231NL...Fl...Scpi...P...KLLLL...AGVD...RLDKD1...254	254
2PL5JA	298N...A...TC...P...FLVVS...YSSDw...LYPPA...217	217
3BF8JA	193A...W...DH...E...ALFIP...GGNsp...VSEQ...212	212
2Y6UJA	262NLLcyMmm...QTfa...R...FLISNvkfvkrktihiv...GARSn...WVPPQ...301	301
2D5LJA	639D...L...KG...R...LMLTH...GALDp...VVVWQ...658	658
2VTVJA	257	saakfasttsnvkaqinvG...A...GS...Natqadydwadg...MPYNAGggdttngvghfrtk...TNTGaiigrmlttctgl...DCAAE...333	333
4G5XJA	206E...A...QL...E...IAVWN...GRDEP...FVELD...225	225
3DDUJA	618N...V...KLpeaddiqyPs...MLLIT...ADHDd...RVVPL...646	646
4QPMJA	232T...I...DA...P...TLILW...YDA...GKQdk...IINVE...251	251
2QM0JA	225T...L...KC...P...VMLVV...GDQA...P...239	239
1HLGJA	303A...M...NV...P...IAVWN...GKQd1...LADPQ...322	322
1LPAJB	191R...L...D...Psdakf...VDVTHtdgapivpnlgfmsqrvv...GHLdfpnggvempgckknlsqIVDIDgiwe...254	254
1AZWJA	252R...Ia...DI...P...GVIVH...GRYDv...VCPLO...272	272
3AZPJA	580R...V...RV...P...FLLLQ...GLEDD...VCPPE...599	599
position		100 110	
1CRLJA	366	fvhasdaEIDTMTaypgditqgspfdtgilnaltppqfkrIsavlgDL.....G..FTlarryflnh...YT..Gg.....TKYsflskqls.....GLPvlgtfhsndivfqdyllgsg	463
2ES4JA	318GV...--	319
3H2GJA	343NAQTAIA.....SFqrgsN...QvaLVdtgtgnasdnasaFA...--H...MLTkesciv...386	386
3QITJA	249DLQQQKM.....Tmt...QA...K..RV...FL..S...GChnlhi...DAaalas1...282	282
3C5WJP	255TIGQMKG.....KF...Q.MQv...LP..Q...CGhavne...DAPdkvaea...286	286
2PL5JA	318QSREIVK.....SLeaadkRV...F..YVv...LQ..Sg...EGHsfill...KNPKqiei...357	357
3BF8JA	213YRDDLA.....QFp...QA...R..AHv...IA..G...AGHwvha...EKPdavira...247	247
2Y6UJA	302NQLFLQK.....TLq...NY...H..LDV...IP..G...GSHlvnv...EAPdlvierinhh...340	340
2D5LJA	659HSLLELD.....ACvka..RTyp...D..YVv...YP..S...HEHnvmpgdr...VHLyet...697	697
2VTVJA	334YT...-T...GP...KA...A..Y...--...--...--...--...--...--...342	342
4G5XJA	226FVSKVKFg...EG...K..Thv...ID..N...AGHapfr...EAPaedday...261	261
3DDUJA	647HSLKFA.....TLgy...IVgrsrkqmnPl.LIh...Vdt.K...AGH...GAGkptakv...688	688
4QPMJA	252VANELKR.....LLk...NA...Qp.Pvi...LE..N...VChkpiL...EAEqlviqq...287	287
2QM0JA	240HEDAVVEcns.....Kldpt...QT...S..FLk...MA..D...SGppql...TOPgkltca...279	279
1HLGJA	323DVGLLp.....Klp...NL...I..YHke...IP..F...YHldfiwam...DAPqevynd...361	361
1LPAJB	255GTRDFAAcnh1r...SYkyyt..DS...-..IVnpdgfag...FPcaSynvftankfcpcpsggcpqMghyadryppgkndvqgkfyldtgdASNfarwrykvsvtlsgkkvtgh	355
1AZWJA	273SAWDLHK.....AWp...KA...Q..LQi...SP..A...SGHsafepenvdalv...RAT...309	309
3AZPJA	600QCDRFLE.....AVagc..GVph...A..YLS...FE..G...EGHfrkrketmvraleaels...LYAqvfgevag...654	654
position		120 130 140	

Fig. S5. Representative sequences of known structure from the MAFFT alignment of 836 α,β -hydrolase fold domains. This corresponds to the same sequences and domain footprint as the GISMO alignment in Fig. S4. In order to emphasize the conserved core columns containing more than 50% deletions in the complete alignment were removed; these correspond to the insert regions shown here.