

Supplemental Material

We selected a set of 300 non-redundant proteins from different families of the PDB, for completeness here we report the list of PDB Ids.

1a5t	1apj	1crk	1f3g	1hme	1lxa	1phh	1srs	1ygs	2pgk	4cat
1a6j	1aqt	1crn	1fbl	1hmy	1mas	1pkp	1sto	1ypt	2pia	4cpa
1a6q	1aua	1cse	1fbp	1hnr	1mat	1pls	1svb	1ytf	2pna	4dfr
1a74	1ay2	1ctf	1fgp	1hoe	1mbb	1pmc	1svq	1yua	2por	4enl
1aa0	1bco	1ctm	1fha	1hp8	1mbn	1png	1tbd	1znf	2prf	4gr
1aa2	1bds	1ctt	1fib	1hpl	1mka	1poi	1tfe	2abk	2sbl	4icd
1aa7	1beo	1cuk	1fkf	1hqi	1mla	1ppr	1tfr	2atc	2sic	4tln
1ab3	1bfm	1cyc	1fmp	1htt	1mmo	1pre	1tim	2bn2	2sns	5acn
1abv	1bgw	1d66	1fmt	1hxp	1msa	1ptq	1tnd	2cab	2spc	5adh
1aca	1bia	1daa	1fps	1hyp	1msk	1pya	1tnf	2cdv	2stv	5rsa
1acc	1bkj	1dch	1fre	1i1b	1nkl	1pyd	1toh	2chs	2taa	7ahl
1acp	1bks	1ddf	1frs	1iba	1nre	1pys	1tpm	2cna	2tpi	9api
1ad2	1ble	1dea	1frv	1ice	1nxb	1qcq	1trk	2cpk	2trt	
1ad3	1bmc	1def	1fsz	1jdw	1nzy	1rbp	1uag	2cpl	2ts1	
1adn	1bp2	1dhy	1fts	1jsg	1occ	1rei	1ubq	2cpp	2tsc	
1adt	1bpl	1div	1fua	1jud	1oen	1rhd	1udg	2cts	2wrp	
1ae9	1bvh	1dkg	1fui	1kbp	1ois	1rie	1utg	2cyp	3eca	
1aep	1bvp	1dkz	1fuq	1knb	1ord	1rla	1vde	2dnj	3fis	
1afp	1bw3	1dms	1gds	1kpt	1osp	1rnt	1vhh	2gbp	3grs	
1ag2	1c5a	1dnp	1gln	1lay	1otf	1rss	1vih	2gls	3icb	
1agr	1cby	1dog	1glu	1lba	1ovo	1sat	1vii	2hgf	3ldh	
1ah7	1cde	1dpr	1glv	1lbd	1pax	1sbt	1vin	2hmg	3mdd	
1ahj	1cfe	1dsb	1gof	1lbe	1pbw	1sei	1vmo	2hmx	3mon	
1aiw	1chc	1ecl	1gpb	1lbu	1pcf	1sig	1vnc	2hpr	3pgm	
1ak1	1chd	1ecr	1gpd	1lci	1pcp	1skn	1vpu	2kau	3pmg	
1alk	1cks	1efn	1gph	1leh	1pda	1slu	1vsg	2lyz	3rub	
1ao6	1cla	1eft	1gpm	1lgh	1pdg	1sly	1whi	2pab	3sdp	
1aol	1cma	1efv	1grl	1lis	1pdo	1smn	1xrc	2pad	4aah	
1aop	1col	1ema	1gss	1lkt	1pdr	1sox	1ycq	2pf2	4ape	
1aor	1coo	1erp	1hip	1lts	1pfk	1spp	1yer	2pgd	4bcl	

Table 1. The PDB Ids of our data set of non-redundant proteins.

In Figure 1 the cluster separation is highlighted by plotting the distribution of distances between the centroids of each cluster and the elements of all 3 clusters.

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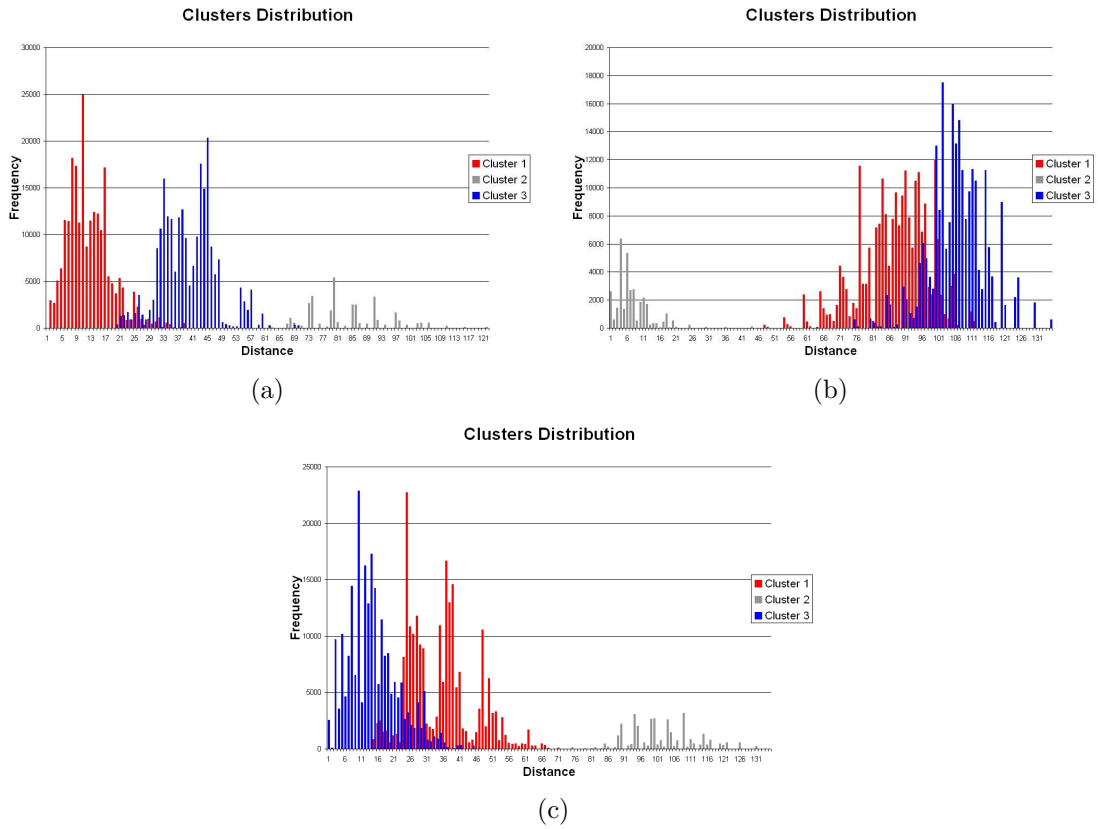


Fig. 1. Distribution of distances from the centroids of each cluster: (a) Cluster 1, (b) Cluster 2, and (c) Cluster 3.