Table S1 Dataset of TIM fold

S No	SCOP ID	Family Name	Abbreviations used	Total members
1	c.1.8.4	Family 1 of glycosyl hydrolase	F1GH	5
2	c.1.8.6	beta-N-acetylhexosaminidase catalytic domain	BNAH	4
3	c.1.8.3	beta-glycanases	BG	11
4	c.1.10.1	Class I aldolase	C1A	3
5	c.1.9.15	PP1699/LP2961-like	PPL	3
6	c.1.2.1	Histidine biosynthesis enzymes	HB	3
7	c.1.8.1	Amylase, catalytic domain	ACD	6
8	c.1.10.5	HMGL-like	HMGL	2
9	c.1.9.1	Adenosine/AMP deaminase	ADA	2
10	c.1.11.2	D-glucarate dehydratase-like	DGDL	6
11	c.1.2.4	Tryptophan biosynthesis enzymes	WB	3
12	c.1.4.1	FMN-linked oxidoreductases	FMNO	6
13	c.1.6.1	Alanine racemase-like, N-terminal domain	ARLN	3
14	c.1.2.3	Decarboxylase	DC	5
15	c.1.12.5	HpcH/HpaI aldolase	HPXA	3
16	c.1.8.8	1,4-beta-N-acetylmuraminidase	BNAM	3
17	c.1.7.1	Aldo-keto reductases (NADP)	AKR	4
18	c.1.12.7	Phosphoenolpyruvate mutase/Isocitrate lyase-like	PEPM	3
19	c.1.8.5	Type II chitinase	T2C	4

The families are aligned such that the top families have electrostatically dominated clusters in the central β- barrel. As one proceeds down the order the dominance of the electrostatics decrease and the dominance of vdW clusters increase.