Table S1 Contacts (hydrogen bonds) provided by the βL residues of two hCC chains creating the dimer. In *italic* distances too long for hydrogen bond formation are marked.

chID:res (atom)	chID:res (atom)	Distance (Å)		
		hCC V57D Aaa = Asp	hCC wt Aaa = Val	hCC V57P Aaa = Pro
A:Gln55 (N)	A':Asn61 (O)	2.95	3.19	2.85
A:Gln55 (O)	A':Asn61 (N)	2.85	3.08	2.83
A:**Aaa**57 (N)	A':Gly59 (O)	2.96	3.42	*4.37*
A:**Aaa**57 (O)	A':Gly59 (N)	3.49	3.46	*5.92*
A:Gly59 (N)	A':**Aaa**57 (O)	3.49	3.46	*5.92*
A:Gly59 (O)	A':**Aaa**57 (N)	2.96	3.42	*4.37*
A:Asn61 (N)	A':Gln55 (O)	2.85	3.08	2.83
A:Asn61 (O)	A':Gln55 (N)	2.95	3.19	2.85

Table S2 Torsion angles φ and ψ calculated using MolProbity program (Lovell *et al.,* 2003*)* for residues from the βL interface of V57D, V57P and the wild-type hCC.

	Torsion angles (^{o})		
	hCC V57D Aaa = Asp	**hCC** Aaa = Val	**hCC V57P** Aaa = Pro
Gln55	-147.4, 127.4	-157.3, 129.1	-153.4, 134.6
Ile56	-86.0, 127.5	-86.6, 130.5	-90.1, 117.1
Aaa57	-142.6, 114.6	-126.8, 153.0	-80.8, 155.1
Ala58	-93.8, 140.4	-135.3, 147.5	-114.0, 71.8
Gly59	-149.4, 166.7	-157.8, -177.4	-115.6, 177.2

Table S3 Superposition of hCC V57P structure on the existing cystatin models, calculated in STRAP (Gille *et al.*, 2001) with TM-align (Zhang *et al.*, 2005). Each comparison is characterized by RMSD (Å) value between the superposed Cα atoms. Explanation of PDB codes: 1G96, two-fold symmetric 3D domain-swapped dimer (Janowski *et al.*, 2001); 1R4C, dimeric form of N-truncated hCC (Janowski *et al.*, 2004); 1TIJ, 3D domain-swapped hCC (Janowski *et al.*, 2005).

	1G96	1R4C (A)	1TIJ (A)	V57P
hCC V57D	0.43	0.72	5.46	0.48
hCC V57P	0.61	0.82	5.39	-