Supplementary Table S2. Solvent accessibility calculations for salt bridge residues.[†]

Table S2a. Total solvent exposed surface area for a single salt bridge at position 286 and 390 for caspase-1 variants (units in $Å^2$).

Construct	Total	Polar	Hydrophobic
Wild type	17.2	12.8	4.4
R286K	18.9	4.8	14.1
E390E	18.1	11.6	6.5
R286K/E390D	17.3	7.7	9.6

Table S2a. Solvent exposed surface area for individual atoms for side chain residues at position 286 and 390 for caspase-1 variants (units in $Å^2$, only atoms with accessible surface area are shown).

Wild type	R286K	E390D	R286K/E390D
Arg286	Lys286	Arg286	Lys286
Cγ – 2.7	Cγ – 2.2	Cγ – 2.9	Cγ – 2.6
Cδ – 0.0	Cδ – 0.0	Cδ – 0.2	Cδ – 1.3
Nε – 2.7	Cε – 7.6	Nε – 2.7	Cε – 0.4
Nη2 – 7.3	Nζ – 0.2	Nη2 – 8.9	Nζ – 5.6
Glu390	Glu390	Asp390	Asp390
Cβ – 0.7	Cβ – 0.8	Cβ – 2.4	Cβ – 4.1
Cγ – 0.0	Cγ – 0.3	Cγ – 1.0	Cγ – 1.2
Cδ – 1.0	Cδ – 3.4		
Oε2 – 2.8	Oε2 – 4.6	Oδ2 – 0.0	Oδ2 – 2.1

[†]These calculations were done using the WHATIF Web Interface based on the following structures: wild type – 2HBQ, R286K - 2H4Y, E390D – 2H4W, R286K/E390D – 2H51.