

S3 Table: Crystallisation conditions

PDB code	Protein variant	Protein details	Treatment	Additions	Crystallisation condition	Temperature
6AZO	SeMet native	4mg/mL in 50 mM tris pH 8 50 mM NaCl 5 mM DTT	chymotrypsin		0.1 M bis-tris chloride pH 6.14 0.089 M lithium sulfate 20.7 %w/v polyethylene glycol 4000	8 °C
6AZN	C175S	13 mg/mL in 50 mM tris pH 7.5 100 mM NaCl	thrombin	5 mM biuret (from 500 mM stock in DMSO)	0.1 M citrate buffer pH 5.5 0.02 M calcium chloride 12 %w/v polyethylene glycol 8000	20 °C
6AZQ	C175S	13 mg/mL in 50 mM tris pH 7.5 100 mM NaCl	thrombin	Saturated biuret in 50 mM tris pH 7.5, 100 mM NaCl	0.1 M citrate buffer pH 5.46 0.027 M calcium chloride 11.9 %w/v polyethylene glycol 8000	20 °C
6AZS	K142A	7 mg/mL in 50 mM tris pH 7.5 100 mM NaCl	thrombin	1 mM N-carbamoyl DL aspartic acid (from 100 mM stock in DMSO)	0.1 M bis tris chloride pH 6.09 23.6 %w/v polyethylene glycol 3350 0.161 M sodium thiocyanate	8 °C
5BK6	K142H	100 mg/mL in 50 mM tris pH 7.5 100 mM NaCl			0.1 M bis tris chloride pH 5.5 17 %w/v polyethylene glycol 10000 0.1 M sodium acetate	20 C