SUPPLEMENTAL DATA

Mutation of Gly11 on the Dimer Interface Results in the Complete Crystallographic Dimer Dissociation of SARS-CoV 3CL^{pro}: Crystal Structure with Molecular Dynamics Simulations

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Running Title: Crystallographic Dimer Dissociation of SARS-CoV 3CL^{pro}

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SUPPLEMENTAL FIGURE LEGENDS

Figure S1. Monomer-monomer interactions mediated by the α-helix A' (residues 10-15) in wild type SARS-CoV 3CL^{pro} dimer (PDB code: 1UK3). The residues involved in the dimer interface are shown as stick models with chain A and B colored in cyan and yellow respectively. The N-terminal finger and α-helix A' are drawn as cartoon, and the hydrogen bonds between α-helix A' residues are displayed explicitly.

Figure S2. CD and fluorescence emission spectra of the Gly11_Ala mutant and wild type SARS-CoV 3CL^{pro}. (a) Far-UV CD spectra of the Gly11_Ala mutant and wild type SARS-CoV 3CL^{pro} at a 10 μM concentration in 10 mM sodium phosphate pH 7.5, 100 mM NaCl at 25 °C (b) Fluorescence emission spectra of the Gly11_Ala mutant and wild type SARS-CoV 3CL^{pro} at 25 °C upon excitation at 280 nm. The samples were prepared in 10 mM Tris-HCl pH 7.5, 100 mM NaCl with a concentration of 3~5 μM. The spectra of the wild type protease and Gly11_Ala mutant are shown in black and light gray, respectively.

Figure S3. The $2F_o$-F_c electron density map around the catalytic dyad in Gly11_Ala monomer. The protein is shown as stick model and the residues are indicated. The distance between His41 and Cys145 is also highlighted. The carbon, nitrogen, oxygen and sulfur atoms are colored in green, blue, red and yellow respectively.

Table S1. Residues involved in the interface between domain III and the rest part of SARS-CoV 3CL^{pro} [a]

1UK3_A		G11A	
Interface area: 771.2 Å^2		Interface area: 696.6 Å^2	
Domain III	Other parts	Domain III	Other parts
Hydrogen bonds		Hydrogen bonds	
ASN 238[O] [b]	THR 199[N]	ASN 238[O]	THR 199[N]
ASN 238[ND2]	ASP 197[O]	ASN 238[ND2]	ASP 197[OD2]
GLU 240[N]	THR 199[O]	ASN 238[ND2]	ASP 197[O]
GLU 288[OE2]	LYS 5 [NZ]	GLU 240[N]	THR 199[O]
ASP 289[OD1]	ARG 131[NH2]	GLU 240[OE2]	ARG 131[NH1]
GLU 290[OE1]	LYS 5 [NZ]	ASP 289[OD1]	LYS 137[NZ]
ASP 295[OD2]	THR 111[OG1]	ASP 289[OD1]	ILE 200[N]
		ASP 289[OD2]	LYS 137[NZ]
		GLU 290[O]	LYS 5 [NZ]
		GLU 290[OE2]	SER 139[N]
		GLU 290[OE1]	SER 139[N]
		GLU 290[OE1]	SER 139[OG]
		ASP 295[OD2]	LYS 5 [NZ]
Salt bridges		Salt bridges	
GLU 288[OE2]	LYS 5 [NZ]	GLU 240[OE2]	ARG 131[NH1]
ASP 289[OD1]	ARG 131[NH1]	ASP 289[OD1]	LYS 137[NZ]
ASP 289[OD1]	ARG 131[NH2]	ASP 289[OD2]	LYS 137[NZ]
ASP 289[OD2]	ARG 131[NH2]	GLU 290[OE2]	LYS 5 [NZ]
GLU 290[OE1]	LYS 5 [NZ]	ASP 295[OD2]	LYS 5 [NZ]
GLU 290[OE2]	ARG 131[NE]		

[a] The interface between domain III and the rest part of the protease was determined by the EBI PISA web server (http://www.ebi.ac.uk/msd-srv/prot_int/picite.html).

[b] Atoms in the parenthesis are those involved in forming the corresponding bonds.

Figure S1

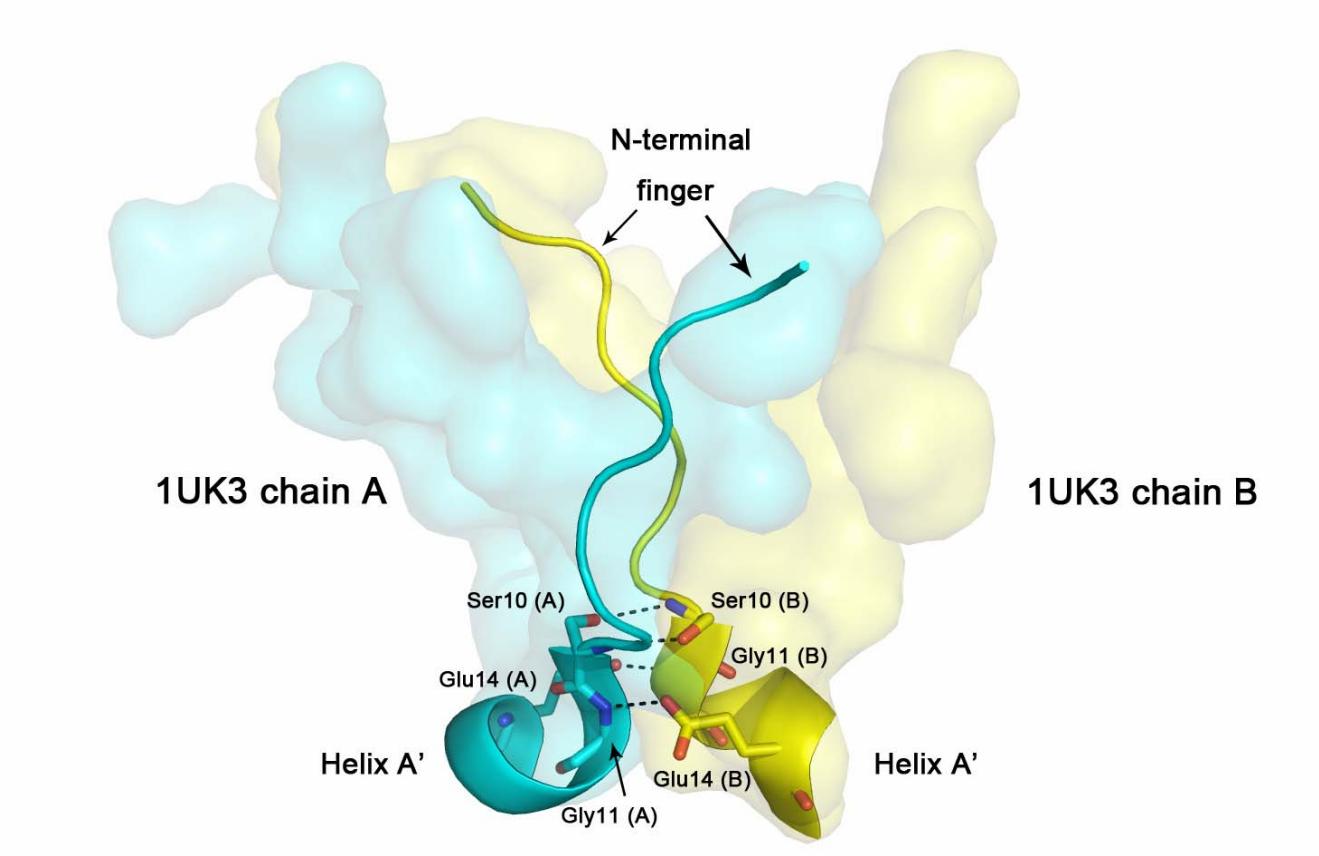
N-terminal
finger
1UK3 chain A
1UK3 chain B
Ser10 (A)
Ser10 (B)
Gly11 (B)
Glu14 (A)
Helix A'
Helix A'
Glu14 (B)
Gly11 (A)

Figure S2

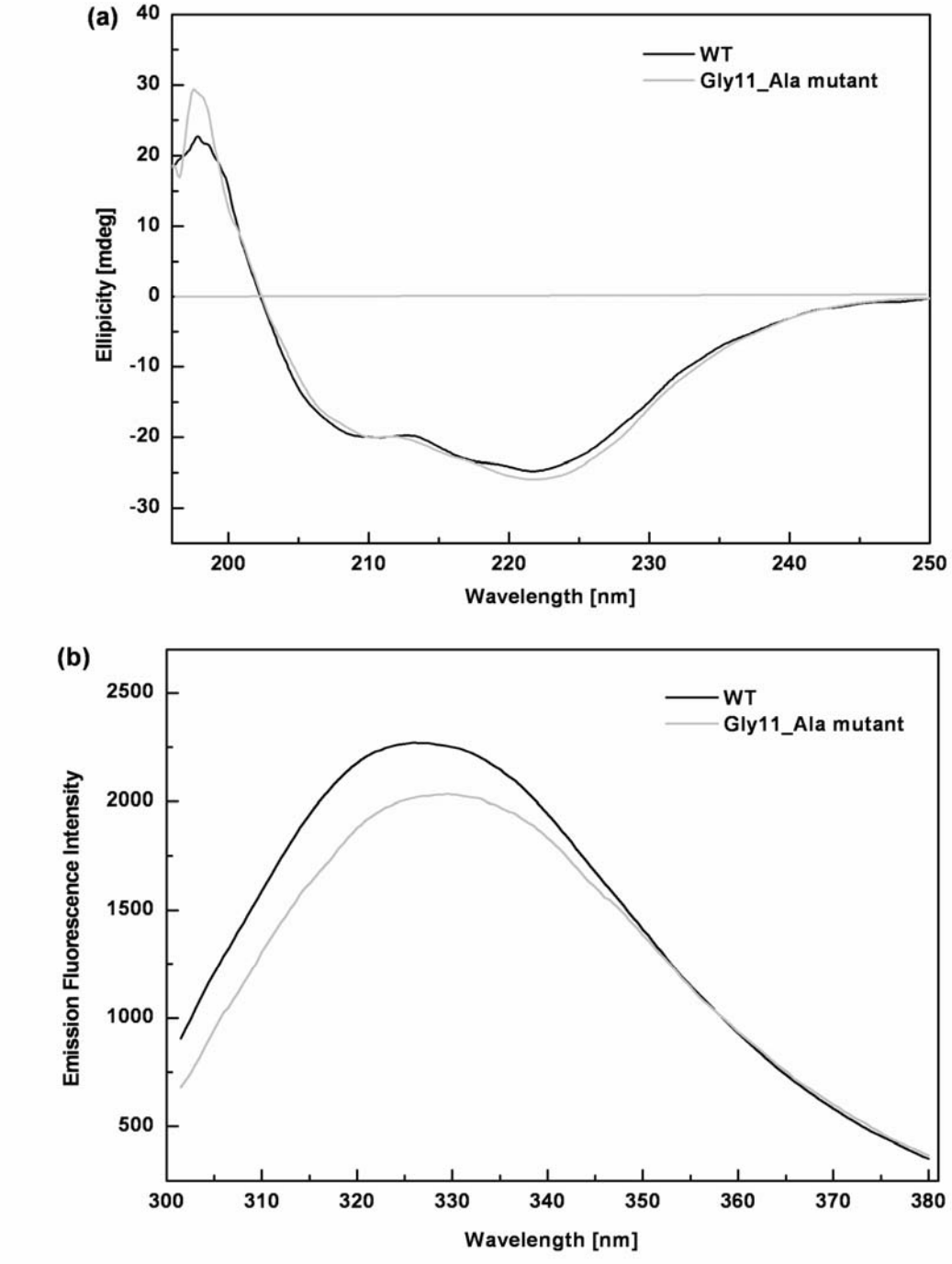
(a)
WT
Gly11_Ala mutant
Ellipicity [mdeg]
Wavelength [nm]
(b)
WT
Gly11_Ala mutant
Emission Fluorescence Intensity
Wavelength [nm]

Figure S3