Table S1. Crystallization, data collection and refinement statistics

Crystallization and data collection						
Name/PDB ids	DvLysin/3m1u		BoYkfC/3npf	BtYkfC/3pvq		BtYkfC/4r0k
Space group	$P2_1$		$P2_12_12_1$	$P2_1$		$P2_1$
Unit cell	*a*=59.3, *b*=54.5, *c*=123.0 Å, *β*=94.1°		*a*=60.1, *b*=62.5, *c*=156.8Å	*a*=64.9, *b*=50.3, *c*=107.6 Å, *β*=93.5°		*a*=65.0, *b*=50.6 *c*=107.9 Å, *β*=93.7°
Beamline	BL9-2		SSRL 9-2	ALS 8.2.2		SSRL 12-2
Data	λ_1 MADSe-inflection	λ_2 MADSe-remote	λ_1 SADSe-peak	λ_1 MADSe-inflection	λ_2 MADSe-remote	λ_1 SADSe-remote
Wavelength (Å)	0.97918	0.91162	0.97925	0.9796	0.9537	1.0000
Resolution range (Å)	29.6-1.75	29.6-1.75	48.9-1.72	29.2-2.10	29.2-2.10	45.8-1.75
No. of observations	251,329	252,636	443,383	98,723	99,008	185,247
No. of unique reflections	78,726	78,779	63,712	40,182	40,250	66,413
Completeness (%)[a]	99.4 (98.3)	99.4 (98.4)	100.0 (100.0)	98.6 (97.1)	98.7 (97.2)	94.0 (94.0)
Mean I/σ (I)[a]	12.5 (2.6)	15.6 (3.1)	14.5 (2.6)	9.6 (2.3)	9.2 (2.2)	10.6 (2.1)
R_{merge} on I[a] (%)	8.7(51.9)	6.3 (43.1)	12.5 (74.7)	10.30 (44.0)	11.0 (46.3)	6.0 (40.6)
R_{meas} on I[a](%)	10.5 (62.7)	7.6 (52.1)	13.5 (81.2)	13.1 (56.2)	14.0 (59.1)	7.3 (51.9)
R_{pim} on I[a] (%)	5.9 (34.9)	4.2 (28.8)	5.0 (31.5)	8.1 (34.5)	8.6 (36.3)	4.1 (32.1)
Highest resolution shell	1.84-1.75	1.84-1.75	1.81-1.72	2.21-2.10	2.21-2.10	1.84-1.75
Model and refinement statistics						
No. of reflections (total)		78,760	63,635		40,234	66,391
No. of reflections (test)		3951	2823		2019	3280
R_{cryst} (%)		13.9	14.1		16.5	15.4
R_{free} (%)		17.3	17.1		19.8	17.7
Stereochemical parameters						
Rmsd bond lengths (Å)		0.015	0.015		0.010	0.010
Rmsd bond angles (°)		1.50	1.46		1.03	0.96
MolProbity score						
All atom clash score		2.8	1.9		2.1	1.2
Ramachandran plot (%)[b]		97.8 (0)	98.2 (0)		99.2 (0)	99.0 (0)
Rotamer outliers (%)		1.2	0.6		1.0	0.6
Average isotropic B-value (Å^2)[c]		20.8 (20.3)	18.5 (16.4)		30.6 (21.8)	31.6 (23.0)
ESU based on R_{free} (Å)		0.10	0.092		0.16	0.092
No. of protein residues / chains in ASU		845/2	602/2		594/2	607/2
Non-protein entities[d]		965	799		455	579

[a]Highest resolution shell in brackets.
[b]Percentage of residues in favored regions of Ramachandran plot (no. of outliers in brackets).
[c]This value represents the total B that includes TLS and residual B components (Wilson B-value in brackets).
[d]Non-protein entities include waters, cryoprotectants, components from the crystallization solutions, and other ions, such as chloride.

ESU = Estimated Standard Uncertainty in coordinates.

$R_{merge}=\Sigma_{hkl}\Sigma_i|I_i(hkl)-\langle I(hkl)\rangle|/\Sigma_{hkl}\Sigma_i I_i(hkl)$

R_{meas}(redundancy-independent R_{merge}) $=\Sigma_{hkl}[N_{hkl}/(N_{hkl}-1)]^{1/2}\Sigma_i|I_i(hkl)-\langle I(hkl)\rangle|/\Sigma_{hkl}\Sigma_i I_i(hkl)$

R_{pim}(precision-indicating R_{merge})$=\Sigma_{hkl}[1/(N_{hkl}-1)]^{1/2}\Sigma_i|I_i(hkl)-\langle I(hkl)\rangle|/\Sigma_{hkl}\Sigma_i I_i(hkl)$.

$R_{cryst}=\Sigma||F_{obs}|-|F_{calc}||/\Sigma|F_{obs}|$, where F_{calc} and F_{obs} are the calculated and observed structure factor amplitudes, respectively.

R_{free} = as for R_{cryst}, but for 5.0% of the total reflections chosen at random and omitted from refinement.