

Table 1. Data collection and refinement statistics

	Vps4 _{122-437,E233Q} Crystal form 1	Vps4 _{104-437,E233Q} Crystal form 2
Data collection		
Space group	P6 ₅ 22	P2 ₁ 2 ₁ 2 ₁
Cell parameters (Å)	a = 110.8 b = 110.8 c = 169.1	a = 77.0 b = 119.8 c = 156.8
Wavelength (Å)	1.00	1.00
Resolution (Å)	30-2.7	30-3.25
Outer Shell (Å)	2.77-2.7	3.37-3.25
Number of Reflections		
Total observed	117,584	121,837
Unique	17,628	23,550
Completeness (%)	99.8 (97.5)	99.8 (100)
R _{sym} (%) ^a	11.1 (52.6)	12.0 (62.9)
Mean I/σ (I)	9.8 (2.3)	8.0 (1.9)
Refinement statistics		
R _{cryst} /R _{free} (%) ^{b,c}	24.1/28.7	21.6/28.9
RMSD from ideal geometry ^d		
Bond lengths (Å)	0.012	0.017
Bond angles (°)	1.489	1.970
Average B-factor (Å ²)	51.5	86.6
Phi/psi angles (non Gly/Pro)		
Most favorable region (%)	86.7	77.4
Additional allowed region (%)	10.7	20.5
Generous allowed region (%)	2.7	1.6
Disallowed region (%)	0.4	0.7

Values in parenthesis are for the highest resolution shell.

^a $R_{\text{sym}} = (|\sum I - \langle I \rangle|) / (\sum I)$, where $\langle I \rangle$ is the average intensity of multiple measurements.

^b $R_{\text{cryst}} = \sum_{\text{hkl}} |F_{\text{obs}}(\text{hkl})| - F_{\text{calc}}(\text{hkl})| / \sum_{\text{hkl}} |F_{\text{obs}}(\text{hkl})|$

^c R_{free} = the crossvalidation R factor for 5% of reflections against which the model was not refined

^d Geometry was analyzed in PROCHECK⁶⁷.