Table 1. Data collection and refinement statistics

Protein	PCSK9
Space group	$P2_12_12_1$
Unit cell parameters, Å	a=62.425 b=70.147 c=148.585
Wavelength, Å	1.0
Resolution range, Å	50.0-1.9
No. unique refs. (observed)	52,284 (208,447)
Completeness, % (highest shell)	99.9(99.9)
R_{merge}, % (highest shell)	7.2 (69.9)
Highest Resolution Shell, Å	1.97-1.9
Mean I/σ(I)	22.5 (2.9)
Refinement	
No. of reflections, total	49,516
No of reflections, test	2,654
R_{cryst} (R_{free}*)[†]	0.19 (0.24)
No. protein atoms	8,677
No. hetero atoms	341
rmsd bonds, Å	0.016
rmsd angles, º	1.52
Average isotropic B-value, Å^2	25.447
ESU based on R_{free}, Å[‡]	0.143

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

[†]$R_{factor} = \Sigma|I_i-\langle I_i\rangle| / \Sigma|I_i|$ where I_i is the scaled intensity of the ith measurement, and $\langle I_i\rangle$ is the mean intensity for that reflection.

[‡]Estimated overall coordinate error (*1*).

1. Tickle IJ, Laskowski RA, Moss DS (1998) *Acta Crystallogr D* 54:243.