Table 1. Data collection and refinement statistics

	PqqC/PQQ
Space group	$P2_12_12$
Wavelength, Å	0.984
Resolution, Å	70-2.3
Reflections (observed)	84,013
Reflections (unique)	24,745
Completeness, % (last shell)	93.4 (89.1)
I/σ (last shell)	8.2 (1.7)
R_{merge}*, % (last shell)	16.2 (42.3)
Resolution range, Å	70-2.3
Reflections (total)	24,745
R_{cryst} †, %	20.51
R_{free} ‡, %	24.83
Protein atoms	4,155
Water molecules	119
rmsd§ angles, °	1.64
rmsd§ bonds, Å	0.017

* $R_{merge} = \Sigma \left| I - \langle I \rangle \right| / \Sigma I$, where I is the observed intensity and $\langle I \rangle$ is the average intensity from multiple observations of symmetry-related reflections. Values in parentheses correspond to the highest resolution shell.

† $R_{cryst} = \Sigma \left| (F_{obs}) - (F_{calc}) \right| / \Sigma (F_{obs})$.

‡ R_{free} = same as R_{cryst} but comprises a test set (5% of total reflections), which was not used in model refinement.

§ rmsd, rms deviation.