Supporting information for Márquez *et al*. (2002) *Proc. Natl. Acad. Sci. USA* **99** (6), 3458–3463. (10.1073/pnas.052461499)

Table 1. Data collection and refinement statistics

Space group		R32		
Unit cell	a b c, Å	152.240	152.240	194.686
	α β γ, °	90.00	90.00	120.00
Data collection				
Resolution, Å		50-1.95 (2.00-1.95)*		
Observations		381,615 (25052)		
Unique reflections		62,908 (4551)		
Completeness, %		99.7 (99.8)		
I/σ		13.5 (4.4)		
R_{sym},† %		8.4 (33.8)		
R_{meas},‡ %		9.1 (37.4)		
Refinement				
Resolution range, Å		50–1.95		
R factor / free R factor,§ %		22.6 / 24.6		
No. of reflections		62,899		
No. of protein atoms in asym. Unit		4,506		
No. of water molecules		293		
No. of ligands, molecules/atoms		9/32		
rmsd bond lengths, Å		0.0056		
rmsd bond angles, °		1.5		
Average B factor, $Å^2$		47.9		

*The number in parentheses refer to the higher resolution shell.

†$R_{sym} = \sum|I_{hi} - I_h| / \sum I_{hi}$, where I_{hi} is the scaled intensity of the *i*th symmetry-related observation of reflection *h* and I_h is the mean value.

‡Redundancy independent R factor as implemented in XDS.

§The free R factor value was calculated using 10% of reflections randomly chosen and not included in the data refinement.