Table 3. Data collection and refinement statistics

	PGRP-IβC	PGRP-IβC–GMPP
Space group	$P2_12_12$	$P2_1$
Unit cell dimensions		
a (Å)	127.4	40.9
b (Å)	56.8	60.9
c (Å)	36.8	97.0
β (˚)		96.5
Resolution (Å)	30–2.2	30–2.1
Observations	215,322	272,478
Unique reflections	12369 (704)*	27,838 (1,328)*
Completeness (%)	91.7 (71.5)	97.9 (96.7)
R_{merge} (%)	8.9 (33.7)	6.4 (27.3)
R_{cryst} (%)	22.9 (31.6)	21.0 (30.7)
R_{free} (%)	28.5 (36.4)	24.2 (34.1)
Molecules per asymmetric unit	2	3
Protein residues	328	502
No. of Ni^{2+} atoms	5	
No. of water molecules	135	325
Average *B* factors (Å^2)		
Protein	23.2	29.6
GMPP		38.4
Waters	31.4	40.1
r.m.s. deviations		
Bonds (Å)	0.019	0.025
Angles (˚)	1.97	2.37
Ramachandran plot statistics		
Core (%)	88.0	91.2
Allowed (%)	11.7	8.8
Generous (%)	0.3	0
Disallowed (%)	0	0

$R_{merge}(I) = (\Sigma|I(i) - \langle I(h)\rangle|/\Sigma I(i))$, where $I(i)$ is the ith observation of the intensity of the *hkl* measurements of the *hkl* reflection. $R_{cryst}(F) = \Sigma_h||F_{obs}(h)| - |F_{calc}(h)||/\Sigma_h|F_{obs}(h)|$ and $|F_{calc}(h)|$ are the observed and calculated structure factor amplitudes for the *hkl* reflection. R_{free} is calculated over reflections in a test set not included in atomic refinement: PGRP-IβC, 654 reflections, 5.0%; PGRP-IβC–GMPP, 670 reflections, 5.1%.

*Values in parentheses correspond to the highest resolution shell: PGRP-IßC (2.3–2.2 Å); PGRP-IßC–GMPP (2.2–2.1 Å).