Supplementary Table 1 Concanavalin A simple truncation using (a) PDB file with waters and (b) PDB file without waters in the model

Resolution(Å)	(a) waters in 2Fo-Fc (1 r.m.s.)	(b) waters in Fo-Fc (2σ)
1.6 waters 11 and 12* waters 13 and 14**	 in density in density	 in density in density
2.3 waters 11 and 12* waters 13 and 14**	 in density in density	 in density in density
3.2 waters 11 and 12* waters 13 and 14**	 no density no density	 in density in density

** waters 11 and 12 are bound to cobalt ion;** waters 13 and 14 are bound to calcium ion.*

Supplementary Table 2 Concanavalin A re-refined at 3.2Å resolution using (a) PDB with waters and (b) PDB without waters in the model

Re-refinements	(a) PDB with waters	(b) PDB without waters
Isotropic restrain: R-factor(%) R-Free factor(%)	 12% 20%	 13% 19%
waters in 2Fo-Fc (0.8 r.m.s)	in density 42*	without density 107
waters in Fo-Fc (2 and 3σ)	in density 77*	without density 72
Common waters**	in density 36 waters	

** included waters 11, 12, 13 and 14;**waters in common between the 2Fo-Fc of the case (a) and the Fo-Fc maps of the case (b).*

Supplementary Table 3 Apocrustacyanin A1 simple truncation using (a) PDB file with waters and (b) PBD file without waters in the model

Resolution(Å)	(a) waters in 2Fo-Fc (1r.m.s.)	(b) waters in Fo-Fc (2σ)
1.4	w93 in density w105 in density	w93 in density w105 in density
2.3	w93 in density w105 in density	w93 in density w105 in density
2.5	w93 in density w105 in density	w93 in density w105 in density
2.7	w93 no density w105 no density	w93 in density w105 in density
2.9	w93 no density w105 no density	w93 no density w105 small density
3.2	w93 no density w105 no density	w93 no density w105 no density

Supplementary Table 4 Apocrustacyanin A1 re-refined using (a) the PDB file with waters and (b) the PDB file without waters in the model at different range of resolutions

Resolutions(Å)	3.2	2.9	2.7	2.5	2.3
(a)					
Isotropic restrain:					
R-factor(%)	18.1%	16.8%	16.9%	17.1%	17.5%
R-Free factor(%)	28.9%	26.2%	24.3%	23.1%	22.4%
waters in 2Fo-Fc (1r.m.s)					
w93	small density	in density	in density	in density	in density
w105	density	in density	in density	in density	in density
(b)					
Isotropic restrain:					
R-factor(%)	20.3%	20.9%	21.8%	22.7%	23.5%
R-Free factor(%)	27.3%	27.0%	27.1%	26.5%	26.4%
waters in Fo-Fc (2σ)					
w93	no density	in density*[1]	in density*[2]	in density*[3]	in density
w105	no density	no density	no density	no density	no density

**water w93 is in density by a shift of (1) 1.23Å (2) 1.03Å (3) 0.60Å.*