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Supporting information for article:

Refinement of Cryo-EM Structures Using Scattering Factors of Charged Atoms

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Supplementary Table 1.

Data collection and refinement statistics

Specimen	catalase	β -galactosidase
Data collection		
Electron 3D crystallography (Yonekura <i>et al.</i> , 2015)		Single particle analysis (Bartesaghi <i>et al.</i> , 2015)
Space group	$P2_12_12_1$	
Cell dimensions		
a, b, c (Å)	69.0, 173.5, 206.0	
α, β, γ (°)	90, 90, 90	
Resolution (Å)	132.7 – 3.2	
Completeness (%)	72.9	
$C_{1/2}$	0.889 (0.779)	
R_{merge}	0.332 (0.334) *	
R_{meas}	0.336 (0.338) *	
R_{pim}	0.044 (0.045) *	
I/σ	15.9 (12.2) *	
Redundancy	46.3 (43.1) *	
Number of crystals	58	
Refinement		
Target function	ML [†]	MLHL [‡]
Resolution (Å)	20 - 3.2	20 - 3.0
Completeness (%)	73.0 (73.0) §	100 (100) ¶
R_{work}	0.2505 (0.2340) §	0.2897 (0.4345) ¶
R_{free}	0.3043 (0.3217) §	
R.m.s deviations		
Bond lengths (Å)	0.007	0.016
Bond angles (°)	0.885	1.641
Ramachandran plot (%)		
Favored	94.0	94.0
Allowed	5.7	5.6
Outliers	0.3	0.4

* Numbers in brackets refer to the highest resolution shell 3.31 – 3.20 Å.

[†] Maximum likelihood (Adams *et al.*, 2010).

[‡] Phased maximum likelihood (Adams *et al.*, 2010).

§ Numbers in brackets refer to the highest resolution shell 3.40 – 3.20 Å.

¶ Numbers in brackets refer to the highest resolution shell 3.19 – 3.00 Å.

Supplementary Table 2.

Parameterization of electron scattering factors of charged and polarized atoms for the 5 Gaussians model*

atom	a ₁ b ₁	a ₂ b ₂	a ₃ b ₃	a ₄ b ₄	a ₅ b ₅	R _{scat} [†] (%)
O ⁻	1.647e+00 4.864e+00	-1.100e+02 1.383e+02	1.058e+02 1.383e+02	-1.281e+01 4.672e+02	-3.965e+01 1.445e+03	0.122
O ^{0.1-}	1.851e+00 6.693e+00	-8.631e-01 2.590e+02	-4.916e+01 1.120e+03	7.505e+01 1.199e+03	-3.133e+01 1.368e+03	0.053
O ^{0.2-}	1.816e+00 6.378e+00	-1.161e+00 1.897e+02	-1.443e+01 7.380e+02	1.814e+01 8.700e+02	-1.366e+01 1.264e+03	0.028
O ^{0.3-}	1.795e+00 6.198e+00	-1.257e+00 1.555e+02	-2.677e+00 4.228e+02	-4.667e+00 9.285e+02	-1.172e+01 1.930e+03	0.016
O ^{0.4-}	1.779e+00 6.059e+00	-1.415e+00 1.392e+02	-2.937e+00 3.606e+02	-6.099e+00 8.101e+02	-1.629e+01 1.857e+03	0.014
O ^{0.5-}	1.748e+00 5.777e+00	1.068e+02 1.487e+02	-1.090e+02 1.487e+02	-6.493e+00 4.850e+02	-1.992e+01 1.470e+03	0.065
O ^{0.6-}	1.727e+00 5.591e+00	1.066e+02 1.452e+02	-1.092e+02 1.452e+02	-7.755e+00 4.788e+02	-2.387e+01 1.462e+03	0.081
O ^{0.7-}	1.706e+00 5.408e+00	1.064e+02 1.427e+02	-1.094e+02 1.427e+02	-9.018e+00 4.745e+02	-2.781e+01 1.456e+03	0.095
O ^{0.8-}	1.687e+00 5.226e+00	1.062e+02 1.408e+02	-1.096e+02 1.408e+02	-1.028e+01 4.715e+02	-3.176e+01 1.451e+03	0.106
O ^{0.9-}	1.667e+00 5.045e+00	1.060e+02 1.394e+02	-1.098e+02 1.394e+02	-1.155e+01 4.691e+02	-3.570e+01 1.448e+03	0.115
Na ¹⁺	1.184e+04 1.443e+01	-1.184e+04 1.443e+01	1.185e+01 2.569e+02	5.547e+01 1.444e+03	3.953e+02 7.977e+03	0.340
Mg ²⁺	2.071e+02 2.137e+01	-2.024e+02 2.137e+01	2.427e+01 2.697e+02	1.116e+02 1.470e+03	7.907e+02 8.013e+03	0.328
Ca ²⁺	-2.167e+04 1.489e+01	2.168e+04 1.489e+01	2.372e+01 2.580e+02	1.109e+02 1.444e+03	7.905e+02 7.976e+03	0.333
Fe ²⁺	5.494e+00 1.084e+01	-1.068e+02 1.764e+02	1.218e+02 1.764e+02	5.907e+01 8.528e+02	2.526e+02 3.550e+03	0.316
Fe ³⁺	6.532e+00 1.324e+01	1.723e+02 1.805e+02	-1.496e+02 1.805e+02	8.897e+01 8.612e+02	3.791e+02 3.563e+03	0.328
H ¹⁺	7.130e-01 -7.900e-03	7.998e+00 1.234e+02	3.724e+01 7.836e+02	1.380e+02 3.444e+03	6.311e+02 1.428e+04	0.004
H ^{0.05+}	4.417e-01 7.807e+00	4.147e-01 9.180e+01	1.428e+01 5.218e+02	-2.560e+01 5.670e+02	1.347e+01 6.508e+02	0.112
H ^{0.1+}	4.482e-01 6.736e+00	6.534e-01 9.562e+01	3.231e-01 2.032e+02	3.925e+00 8.274e+02	1.417e+03 6.870e+03	0.078
H ^{0.2+}	4.726e-01 5.229e+00	1.299e+00 1.056e+02	4.753e-01 1.905e+02	7.686e+00 8.074e+02	1.058e+03 5.988e+03	0.048
H ^{0.3+}	4.983e-01 4.030e+00	1.937e+00 1.097e+02	6.233e-01 1.780e+02	1.141e+01 7.986e+02	1.815e+02 4.531e+03	0.033
H ^{0.4+}	5.193e-01 2.905e+00	6.497e-01 8.940e+01	2.658e+00 1.308e+02	1.484e+01 7.852e+02	2.674e+01 2.970e+03	0.026

* Calculated from data up to $2 \sin \theta / \lambda = 1 / 2 \text{ \AA}^{-1}$.

[†] Defined in equation (1).