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Supporting information for article:

Automated identification of elemental ions in macromolecular crystal structures

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Table S1 Parameters and default tolerances for cation identification. These are also available in machine-readable form in CCTBX in the file mmtbx/ions/ion_parameters.cif. Tables S1 and S2 were based in part on Rulísek & Vondrásek 1998; Harding 2000, 2001; Muller et al. 2003; Dokmanic et al. 2008; Zheng et al. 2008.

Ion	VECSUM (max)	# of coordinating atoms	Minimum # of non-water coordinating atoms	Bond valence sum (upper and lower bounds)
Na^{+}	0.4	4-8	1	0.8-1.2
Mg^{2+}	0.4	4-6	0	1.8-2.2
K^{+}	0.4	4-8	1	0.8-1.2
Ca^{2+}	0.4	5-8	0	1.75-2.2
Mn^{2+}	0.4	4-6	1	1.75-2.2
Fe^{2+}	0.4	5-6	1	1.75-2.2
Co^{2+}	0.4	5-6	1	1.75-2.2
Cu^{2+}	0.4	3-4	1	1.75-2.2
Ni^{2+}	0.4	4-6	1	1.75-2.2
Zn^{2+}	0.4	4-6	1	1.75-2.4
Cd^{2+}	0.6	3-7	1	1.5-2.3

Table S2 Additional filtering criteria for cations.

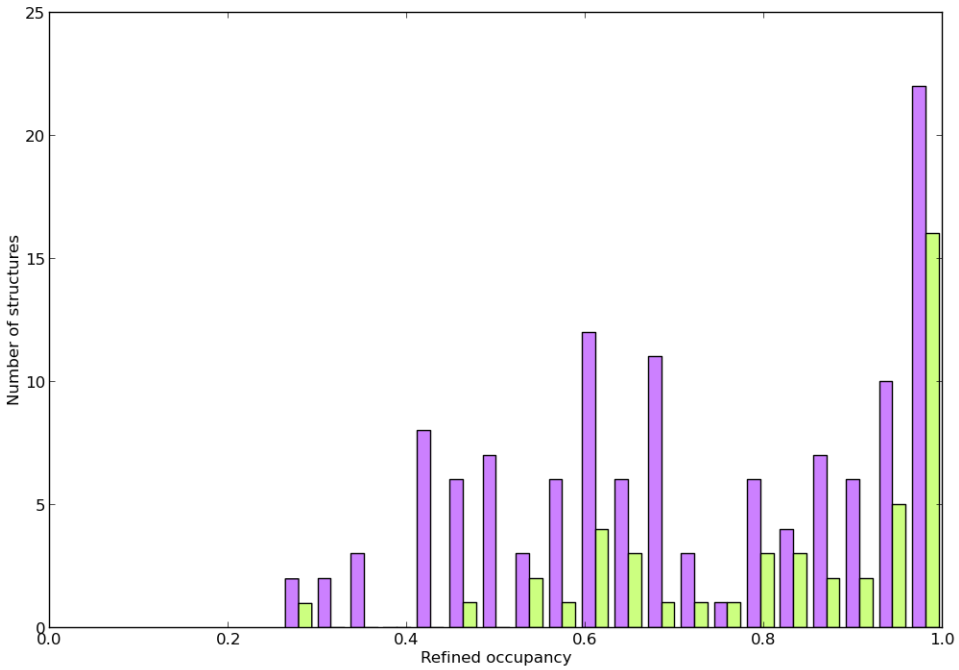
Ion	Coordinating atoms	Coordinating protein sidechains	Geometry	Coordinating protein backbone atoms
Na^{+}	O	Any with oxygen atoms	Octahedral, square-pyramidal, none	O, OXT
Mg^{2+}	O, N	Ser, Thr, Asp, Asn, Glu, Gln, His	octahedral	O, OXT
K^{+}	O	Any with oxygen atoms	any	O, OXT
Ca^{2+}	O	Any with oxygen atoms	Octahedral, pentagonal-bipyramidal, none	O, OXT
Mn^{2+}	O, N	Ser, Thr, Asp, Asn, Glu, Gln, His	any	-
Fe^{2+}	O, N, S	Cys, Asp, Glu, His, Tyr	any	-
Co^{2+}	O, N	Cys, Asp, Glu, His	Tetrahedral, octahedral	-
Cu^{2+}	O, N, S	Cys, Met, His	Tetrahedral, square planar, none	-
Ni^{2+}	O, N, S	Cys, Asp, Glu, His	Tetrahedral, octahedral, None	-
Zn^{2+}	O, N, S	Cys, Asp, Glu, His	Tetrahedral, octahedral, none	-
Cd^{2+}	O, N, S	No restrictions	Tetrahedral, octahedral, none	O, OXT

Table S3 Individual structures in the JCSG blind set.

PDB ID	Resolution (Å)	Ions	Notes
2fm1	2.25	2 CA	
2gf6	1.91	1 CA	
2gvi	1.87	5 ZN	(Axelrod, Das et al. 2010)
2qpx	1.40	2 ZN	
3cjy	1.70	1 CA	
3db7	1.40	3 CA	
3dzz	1.61	2 CA	
3fd0	2.12	1 CA	
3g0k	1.30	1 CA	
3h50	1.60	4 ZN	(Axelrod, Kozbial et al. 2010)
3jtx	1.91	1 CA	
3ju7	2.19	4 CA	
3llx	1.50	1 ZN	
3lub	12.11	12 CA, 24 ZN	
3luu	1.93	1 ZN	
3lwu	2.10	1 ZN	
3m83	2.12	8 CA	(Levisson et al. 2012)
3mbj	2.10	3 ZN	
3mcx	1.49	6 ZN	
3mdo	1.91	7 CA	
3mzo	1.98	11 CA	1 alt. conf.
3n91	2.40	1 CA	
3na6	2.00	1 CA	
3nqn	1.88	3 CA	
3o14	1.70	2 ZN	
3ohe	1.20	3 CA	1 alt. conf.
3oqq	2.08	4 CA	
3orj	2.16	1 ZN	
3oru	1.11	1 ZN	
3p1v	1.93	4 ZN	

3pfo	1.90	4 ZN	two of these appear to be something lighter (no anomalous)
3pgv	2.39	4 CA	
3pw3	2.23	6 ZN	
3qc0	1.45	1 ZN	annotated as partial (or mixed) occupancy
3qov	2.20	4 ZN	
3qta	2.00	3 CA	
3r4i	2.24	13 CA	
3s6f	1.19	2 CA	
3son	1.71	2 CA	
3tc8	1.06	2 ZN	
3u1w	2.00	4 CA	
3u7z	1.30	14 CA	2 alt. confs.
3urz	2.19	4 ZN	
4dgu	2.37	9 ZN	
4e5v	1.75	2 ZN	
4e6r	2.20	5 ZN	
4ecg	2.30	9 CA	
4epz	1.68	2 CA	
4esn	2.20	2 ZN	
4f53	2.25	3 CA	
4iej	1.30	1 CA	
4fuu	1.45	1 ZN	
4leh	2.90	1 ZN	
4lqx	2.34	2 ZN	

Figure S1 Histograms of refined occupancies for (A) calcium ions and (B) zinc ions in the JCSG "blind" test set. Purple bars represent statistics for the deposited structures re-refined in *phenix.refine*; green bars represent statistics only for the ions that could be identified correctly. X-axes (but not y-axes) are on the same scale in both plots.



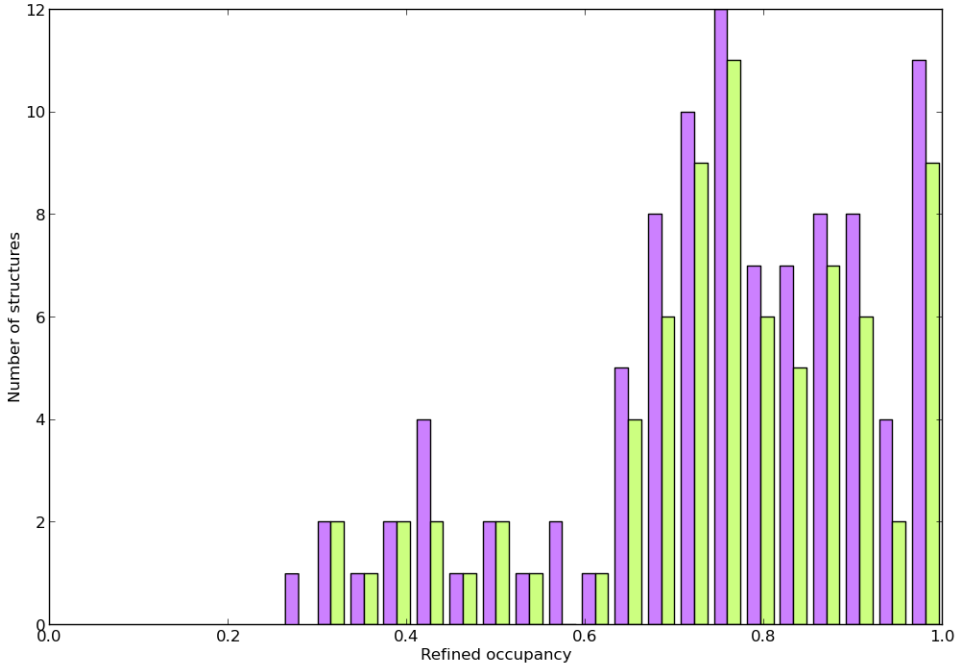


Figure S2 Histograms of normalized refined total isotropic equivalent B-factors for (A) calcium ions and (B) zinc ions in the blind test set, calculated by dividing the ion B-factor by the mean for all non-hydrogen atoms in a given structure. Colors are as in Figure S1.