

# Naked metal cations swimming in protein crystals

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## Supplementary Material

**Table S1.** The following quantities are reported for each cation: The total number of occurrences in the Protein Data Bank (Total number), the occurrences in which the cation is naked (Naked) and the percentage of naked cations (% naked). The numbers in parentheses are the number occurrences computed as the sum of the occupancy values deposited in the Protein Data Bank.

Cation	Total number	Naked	% naked
Li	136 (132)	4 (4)	3 (3)
Na	23342 (22810)	1826 (1786)	8 (8)
K	7312 (6607)	1368 (1309)	19 (20)
Rb	250 (131)	35 (22)	14 (17)
Cs	412 (237)	267 (187)	65 (79)
Fr	0 (0)	0 (0)	-nan (-nan)
Be	405 (398)	0 (0)	0 (0)
Mg	61887 (60495)	10434 (10252)	17 (17)
Ca	31968 (30986)	1061 (1013)	3 (3)
Sr	1428 (1373)	822 (815)	58 (59)
Ba	296 (173)	140 (117)	47 (68)
Ra	0 (0)	0 (0)	-nan (-nan)
Sc	1 (1)	0 (0)	0 (0)
Ti	3 (3)	1 (1)	33 (33)
V	397 (355)	0 (0)	0 (0)
Cr	17 (17)	0 (0)	0 (0)
Mn	11352 (10773)	959 (932)	8 (9)
Fe	36809 (35486)	63 (46)	0 (0)
Co	2786 (2515)	125 (100)	4 (4)
Ni	3583 (3271)	130 (108)	4 (3)
Cu	6147 (5279)	20 (13)	0 (0)
Zn	36327 (34102)	290 (236)	1 (1)
Y	193 (162)	16 (14)	8 (9)
Zr	33 (30)	1 (1)	3 (3)

Nb	0 (0)	0 (0)	-nan (-nan)
Mo	955 (749)	57 (24)	6 (3)
Tc	0 (0)	0 (0)	-nan (-nan)
Ru	269 (174)	2 (1)	1 (1)
Rh	50 (28)	0 (0)	0 (0)
Pd	114 (84)	3 (1)	3 (1)
Ag	98 (91)	3 (2)	3 (2)
Cd	4706 (3665)	138 (108)	3 (3)
La	20 (17)	1 (1)	5 (6)
Hf	44 (43)	0 (0)	0 (0)
Ta	206 (79)	0 (0)	0 (0)
W	702 (532)	89 (50)	13 (9)
Re	88 (58)	5 (1)	6 (2)
Os	34 (26)	33 (28)	97 (108)
Ir	146 (63)	29 (23)	20 (37)
Pt	614 (300)	81 (42)	13 (14)
Au	333 (174)	85 (46)	26 (26)
Hg	1840 (1122)	118 (68)	6 (6)
Ce	4 (2)	0 (0)	0 (0)
Pr	64 (48)	10 (7)	16 (15)
Nd	0 (0)	0 (0)	-nan (-nan)
Pm	0 (0)	0 (0)	-nan (-nan)
Sm	164 (135)	25 (19)	15 (14)
Eu	72 (39)	0 (0)	0 (0)
Gd	255 (156)	24 (10)	9 (6)
Tb	138 (98)	8 (4)	6 (4)
Dy	30 (10)	0 (0)	0 (0)
Ho	37 (30)	0 (0)	0 (0)
Er	10 (10)	1 (1)	10 (10)
Tm	0 (0)	0 (0)	-nan (-nan)
Yb	215 (162)	29 (15)	13 (9)
Lu	52 (32)	14 (12)	27 (38)
Al	361 (358)	0 (0)	0 (0)
Ga	15 (15)	0 (0)	0 (0)
Ge	0 (0)	0 (0)	-nan (-nan)
In	1 (1)	0 (0)	0 (0)
Sn	19 (14)	0 (0)	0 (0)

Sb	8 (6)	1 (1)	12 (17)
Te	27 (14)	1 (1)	4 (7)
Tl	168 (68)	23 (11)	14 (16)
Pb	159 (108)	31 (15)	19 (14)
Bi	3 (1)	0 (0)	0 (0)