

Supplementary information for

Novel insights into nickel import in *Staphylococcus aureus*: positive role of free histidine and structural characterization of a putative thiazolidine-type nickelophore

Hugo Lebrette^a, Elise Borezée-Durant^b, Lydie Martin^a, Pierre Richaud^{c,d,e}, Elisabetta Boeri-Erba^a and Christine Cavazza^{f,g,h*}

Table 1: Data collection and refinement statistics for SaNikA structures.

	SaNikA-LB	SaNikA-M9	SaNikA-M9/Ni(His) ₂	SaNikA-BHI	SaNikA-CD	SaNikA-CDΔHis
PDB ID code	4OFJ		4XKN	4XKP	4XKQ	4XKR
Data collection						
Beamline	ID29 (ESRF)	ID29 (ESRF)	BM30A (ESRF)	ID29 (ESRF)	ID14eh4 (ESRF)	ID29 (ESRF)
Wavelength (Å)	0.98400	0.98400	0.979621	0.97901	1.00446	0.97625
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell parameters	a = 61.90 Å b = 67.72 Å c = 115.65 Å α = β = γ = 90°	a = 124.15 Å b = 118.78 Å c = 164.64 Å β = 105.313°	a = 62.49 Å b = 67.20 Å c = 115.53 Å α = β = γ = 90°	a = 62.34 Å b = 67.24 Å c = 115.21 Å α = β = γ = 90°	a = 62.50 Å b = 67.22 Å c = 116.04 Å α = β = γ = 90°	a = 61.80 Å b = 67.37 Å c = 115.57 Å α = β = γ = 90°
Resolution range (Å)	45.69-1.70 [1.80-1.70]	49.14-4.0 [4.10-4.00]	45.76-1.85 [1.95-1.85]	45.72-1.90 [2.00-1.90]	45.77-1.90 [2.00-1.90]	45.54-1.75 [1.80-1.75]
<i>R</i> _{sym} (%)	7.9 [65.2]	21.9 [113.9]	11.1 [66.9]	12.0 [71.4]	11.1 [79.9]	7.8 [61.6]
<i>I</i> /σ	17.04 [4.23]	8.17 [1.65]	16.89 [2.94]	13.13 [2.58]	13.60 [3.14]	14.6 [3.36]
Completeness (%)	99.6 [99.4]	85.8 [75.6]	99.8 [99.2]	99.9 [99.9]	99.4 [97.7]	96.6 [96.4]
Redundancy	7.2 [7.4]	5.7 [5.6]	7.0 [6.0]	7.3 [7.1]	6.2 [6.2]	4.4 [4.5]
<i>N</i> _{measured}	390110 [61952]	191505 [11786]	295789 [36402]	284125 [38639]	242226 [33324]	208978 [17007]
<i>N</i> _{unique}	53990 [8368]	33704 [2088]	42182 [6050]	38955 [5455]	39047 [5392]	47766 [3799]
Refinement						
<i>R</i> factor/ <i>R</i> _{free} factor (%)	14.8/18.5		15.0/19.2	15.8/19.1	15.5/19.5	17.2/20.5
No. protein atoms	3780		3763	3802	3802	3765
No. ligand atoms	140		140	92	98	145
No. water molecules	415		496	415	365	397
average B-factor (Å ²)	23.1		21.2	23.8	24.7	21.4
Rmsd bonds (Å)	0.015		0.008	0.007	0.010	0.013
Rmsd angles (°)	1.56		1.11	1.07	1.25	1.50
Ramachandran plot:						
Residues in most favorable regions (%)	97.5		97.7	97.9	97.9	96.8
Residues in allowed region (%)	2.5		2.3	2.1	2.1	2.7
Residues in disallowed region (%)	0		0	0	0	0.5