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Supporting information for article:

Serendipitous crystallization and structure determination of bacterioferritin from *Achromobacter* species

Abhisek Dwivedy, Bhavya Jha, Khundrakpam Herojit Singh, Mohammed Ahmad, Anam Ashraf, Deepak Kumar and Bichitra Kumar Biswal

>>tr|A0A0M7NRX6| Bacterioferritin OS=Achromobacter sp.
MKGDKTVIQFLNKQLTNELTAINQYFLHARMLNHWGFDKLGKHEYEESIGEMKHADRLIARIFMLDGLPNLQDLHKLL
IGEDVPELLACDLKLEQGAQATVKEAIAYCESVRDYVSRDLF QDILDDTEEHIDYLETQIDLIDKVGLQNYLQSQMSVPD

Coverage- 82.8 %	Unique peptides -16	
Mass	Score	Accessions
18290	670	gi|918212572

Figure S1 MALDI-TOF MS/MS analysis confirming the identity of *Ach* Bfr. 16 unique peptides were identified by mass fingerprinting and the MASCOT analysis revealed multiple hits including the A0A0M7NRX6, the general amino acid sequence for *Achromobacter* Bfr.

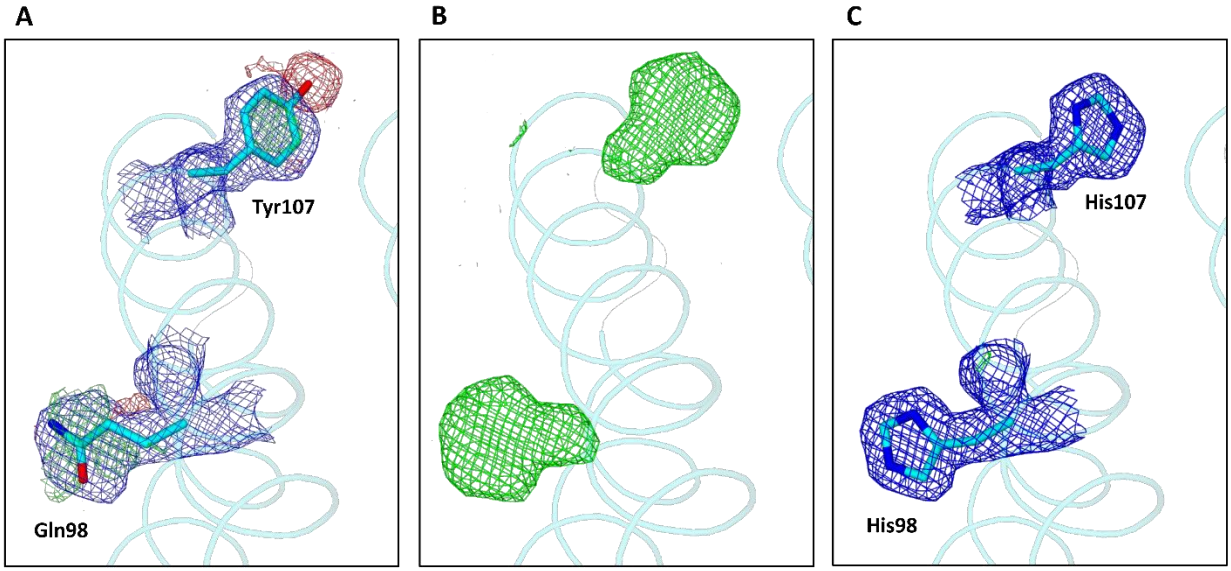

Figure S2 Identification of the amino acids unique to DH1f species Bfr sequence. **(A)** The pronounced disagreement between $|F_o|$ - $|F_c|$ (2.5σ and -3σ) and $2|F_o|$ - $|F_c|$ (1σ) electron density peaks for residues-Gln98 and Tyr107 is depicted. **(B)** An unbiased $|F_o|$ - $|F_c|$ (2.5σ) was obtained for side chains of residues 98 and 107 after restricting the said residues to Cα followed by refinement. The map clearly indicates the presence of His side chains at both these positions. **(C)** No residual difference electron density peaks (2.5σ) were observed after incorporating His at 98 and 107 positions while the residues fit perfectly in $2|F_o|$ - $|F_c|$ peaks. The $|F_o|$ - $|F_c|$ peaks are depicted either in green (2.5σ) or in red (-3σ) and the $2|F_o|$ - $|F_c|$ peaks are shown in blue color.

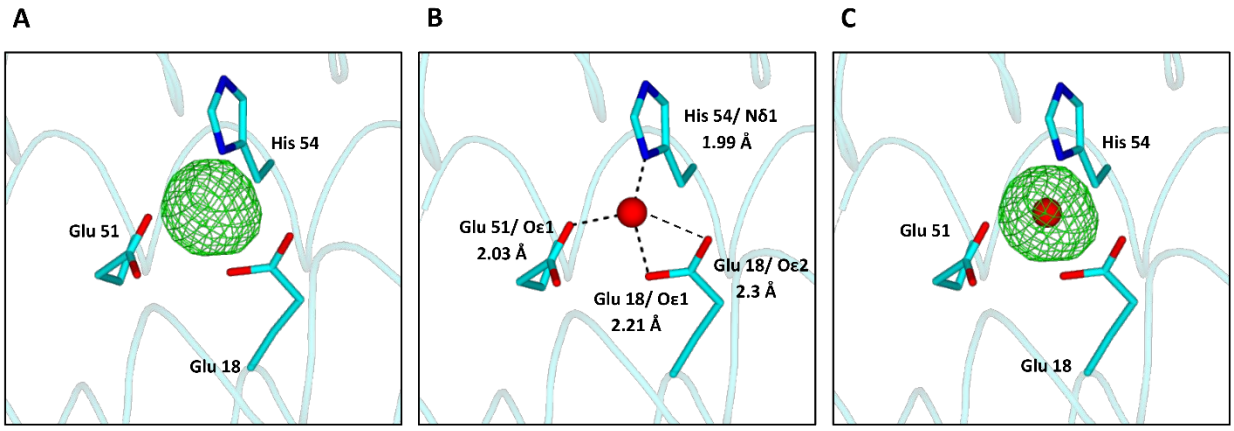

Figure S3 Presence of a single Fe^{II} ion at the iron storage site in *Ach* Bfr. **(A)** A distinct $|F_o|$ - $|F_c|$ spherical electron density peak (contoured at 5.0σ) was observed in each monomer of *Ach* Bfr at the usual iron storage site reported for Bfrs, indicating the presence of a metal atom. **(B)** No residual difference electron density peak (2.5σ) was observed after incorporating Fe^{II} in that position. **(C)** The final refined Fe^{II} was superimposed on the electron density map. In all cases, $2|F_o|$ - $|F_c|$ electron density peaks (at 1σ) were observed. Residues His54, Glu51, Glu18 are shown in sticks and Fe^{II} is depicted as red sphere.