Supplementary Figure 1 Fourier Shell Correlation for cryoEM reconstruction of OmcS filament.

Fourier Shell Correlation



Supplementary Figure 2

OmcS in relation to other multi-heme cytochromes. 1z1n is a branched 16-heme cytochrome from Desulfovibrio gigas¹, while the others are from Geobacter sulfurreducens: 30v0 - 12-heme cytochrome c², 3bxu - 3-heme cytochrome c³, 10s6 - 3-heme cytochrome c7⁴, 3h33 - 3-heme cytochrome c7⁵, OmcS (pdb: 6nef) - 6-heme cytochrome.



Supplementary Figure 3 OmcS shown with the thickness of the tube related to the b-factor of the model in that area. This reflects the areas in the model where the fit to the density contained the most uncertainty.



Supplementary Figure 4

(A) The heme centers overlayed on the density map at high threshold (coloured purple for clarity). (B) at lower threshold the heme centers cover the core of each porphyrin. The histidines that coordinate the iron are evident as densities perpendicular to the porphyrin planes. (C) The putative magnesium ion is coordinated by heme504.



Supplementary Table 1 In Supplementary Table: Closest interatomic contacts between neighbouring hemes, inter-iron distances, and angles between heme planes.

Heme	Atom	Heme	Atom	Distance (Å)	Fe-Fe	Inter-heme	
					Distance (Å)	angle [degrees]	
501	CBC	502	CHC	4.0	13.0	71.4	
502	C3A	503	CMA	3.5	9.3	176.9	
503	CBC	504	CHC	3.9	11.2	67.6	
504	C2A	505	CMA	3.2	9.3	175.1	
505	CBC	506	CAB	4.1	11.3	96.5	
506	O2A	501	CAA	3.4	9.0	168.8	

Supplementary Table 2: Inductively coupled plasma mass spectrometry (ICP-MS)

		Concentration, mg/kg												
		SD		SD		SD		SD		SD		SD		
Sample Name	Fe	(Fe)	Mg	(Mg)	K	(K)	Ca	(Ca)	Mn	(Mn)	Zn	(Zn)	Sr	SD(Sr)
Sample W	< 0.005		< 0.01		< 0.02		< 0.01		< 0.002		< 0.002			< 0.002
Sample B	0.049	0.005	< 0.01		0.12	0.01	< 0.01		0.0029	0.0003	< 0.002			< 0.002
Sample B+W	0.104	0.003	< 0.01		< 0.02		< 0.01		0.0028	0.0003	< 0.002			< 0.002
Sample G Sulf Pili	1.47	0.02	0.61	0.02	0.41	0.02	0.24	0.01	0.0125	0.0006	0.01	0.001	0.0046	0.0005

sample w = milli-Q water directly from our system

sample b = 150mM Ethanolamine, pH 10.5 made using Ethanolamine-HCl plus NaOH.

sample w + b = 150mM Ethanolamine, pH 10.5 dialyzed against milli-Q water

References

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