

SUPPLEMENTAL INFORMATION

Figure legends

Figure S1- Amino acid sequence alignment of *Acidianus ambivalens* SQR (acession numbers in parentheses) with sulfide:quinone oxidoreductases from Group I. Aambivalen, *Acidianus ambivalens* (CAD33806.1); Stokodaii, *Sulfolobus tokodaii str. 7* (NP_378484.1); Ssolfatari, *Sulfolobus solfataricus* P2 (NP_343636.1); Picophilu, *Picrophilus torridus DSM 9790* (YP_023317.1), Tacidophilu, *Thermoplasma acidophilum DSM 1728* (NP_394588.1), Telongatus, *Thermosynechococcus elongatus* BP-1 (NP_681079.1), Aaeolicus, *Aquifex aeolicus VF5* (NP_214500.1), Rcapsulatu, *Rhodobacter capsulatus* (CAA66112.1), Olimnetica, *Oscillatoria limnetica 'Solar Lake'* (AAF72962.1), Mferrooxyd, *Mariprofundus ferrooxydans PV-1* (ZP_01453072.1).

Figure S2 – Anomalous difference Fourier map showing the continuous electron density bridging the two redox active site cysteins. The map was calculated with a dataset collected at 1.711 Å wavelength and is contoured at 3.5σ .

Figure S3 – Schematic representation of the putative C-terminal amphipatic helix proposed to be involved in membrane attachment (residues 385-409).

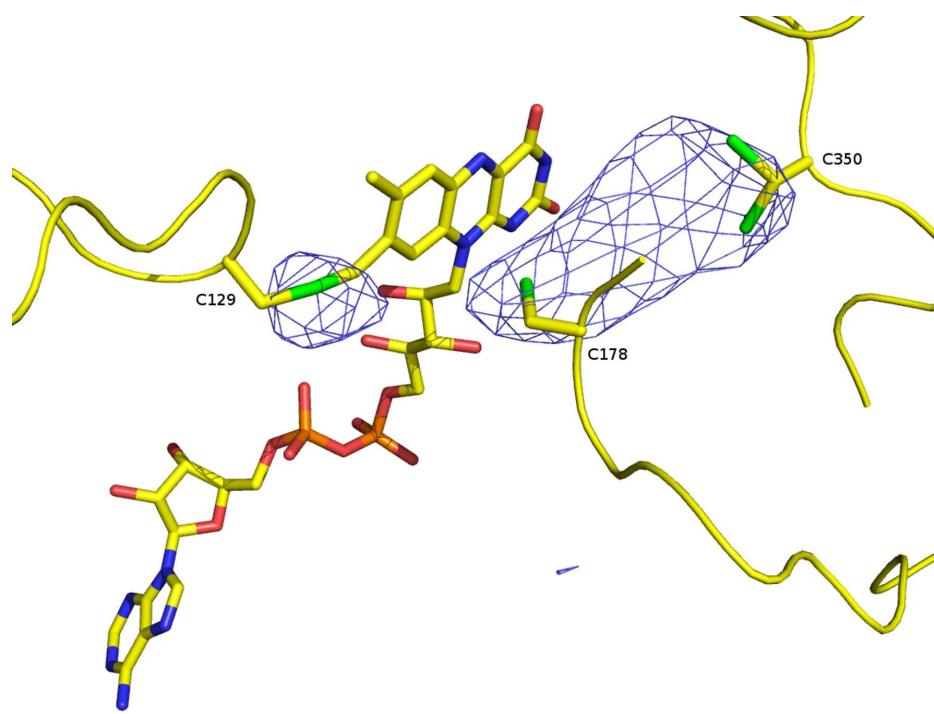
Table legends

Table S1 – Data collection and refinement statistics (values between parentheses refer to the last resolution shell)

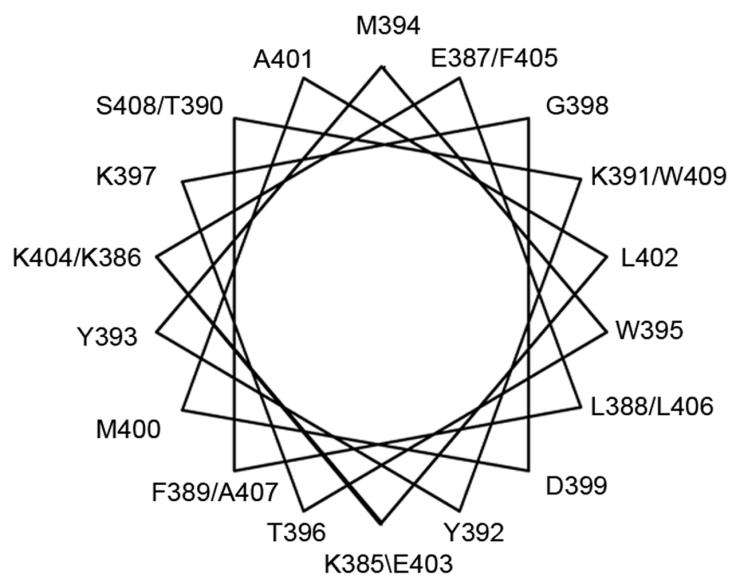
Structure and function of sulfide:quinone oxidoreductase

Figures

Brito *et al* Figure S1



Brito *et al* Figure S2



Brito *et al* Figure S3

Table S1

Table S1 – Data collection and refinement statistics (values between parentheses refer to the last resolution shell)

| | SQR _T | SQR |
|---|-----------------------|-----------------------------------|
| Space group | | P6 ₅ 22 |
| Unit cell | | |
| <i>a=b</i> , <i>c</i> (Å) | 178.6, 162.3 | 179.7, 163.4 |
| Data collection* | | |
| Beamline | | ESRF ID14-1 |
| Wavelength (Å) | | 0.934 |
| Resolution range (Å) | 47.43-2.65 (2.80-2.7) | 51.44-2.57 (2.71-2.6) |
| Total no. of observations | 157117 | 383076 (29746) |
| No. of unique observations | 44293 (6392) | 49511 (6870) |
| R _{merge} * (%) | 8.2 (50.4) | 7.5 (51.0) |
| R _{pim} # (%) | 11.3 (35.9) | 8.5 (30.3) |
| Completeness (%) | 99.6 (99.9) | 99.5 (96.8) |
| Mean <I / σ(I)> | 10.2 (2.0) | 20.0 (2.6) |
| Refinement statistics | | |
| R _{work} / R _{free} (%) | 19.6 / 22.5 | 19.4 / 22.2 |
| Geometry | | |
| rms bonds (Å) | 0.006 | 0.006 |
| rms angles (°) | 0.907 | 0.892 |
| Residues included | | T ₂ - E ₃₅₇ |
| Ramachandran statistics | | |
| Residues in most favored regions (%) | 94.9 | 96.3 |
| Residues in allowed regions (%) | 4.4 | 3.0 |
| Residues in disallowed regions (%) | 0.7 | 0.7 |
| Mean B factors | | |
| Protein (Å ²) | 56.8 | 55.4 |
| FAD (Å ²) | 49.4 | 46.6 |
| PS3 (Å ²) | 61.0 | 57.8 |
| Solvent (Å ²) | 61.0 | 61.3 |

$$^* R_{\text{merge}} = \sum_{hkl} \sum_i |I_i(hkl) - \overline{I(hkl)}| / \sum_{hkl} \sum_i I_i(hkl)$$

Structure and function of sulfide:quinone oxidoreductase

$$\# R_{pim} = \sum_{hkl} \left[\frac{1}{N-1} \right]^{1/2} \sum_i |I_i(hkl) - \overline{I(hkl)}| / \sum_{hkl} \sum_i I_i(hkl)$$

Calculated with the program SCALA, R_{merge} and R_{pim} are indicators of the precision of the final merged and averaged data-set, where $I_i(hkl)$ is the observed intensity of the i^{th} measurement, $\overline{I(hkl)}$ is the average intensity of multiple observations of symmetry-related reflections and N is redundancy.

Brito *et al* Table S1