# Dissecting the mechanism of oxygen trafficking in a metalloenzyme

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## Electronic Supplementary Data

5 **Table S1** Crystallographic Data Collection and Refinement

|  | I342F[b] | E490A[c] | E490I[b] | E490Q[c] |
|---|---|---|---|---|
| **Data Collection** |  |  |  |  |
| Wavelength (Å) | 0.9796 | 1.5418 | 1.5418 | 1.5418 |
| Space Group | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ |
| Cell dimensions, $a,b,c$ (Å) | 79.1, 133.9, 166.6 | 80.2, 135.2, 167.6 | 80.0, 135.4, 166.8 | 80.1, 135.1, 167.1 |
| Resolution (Å) | 45-2.30 (2.42-2.30)[a] | 62.7-2.35 (2.43-2.35) | 51.3-2.00 (2.11-2.00) | 71.1-2.1 (2.2-2.1)) |
| $R_{merge}$ (%) | 10.7 (40.4) | 12.4 (34.5) | 5.9 (47.1) | n.a[d] |
| $R_{p.i.m.}$ (%) | 4.3 (16.0) | n.d | 3.2 (44.3) | n.a |
| $<I>/sd<I>$ | 17.3 (4.6) | 6.6 (3.2) | 14.8 (1.2) | n.a |
| Completeness | 100 (100) | 81.9 (83.6) | 77.7 (55.7) | 93.2 (65.4) |
| Multiplicity | 7.3 (7.3) | 2.75 (2.58( | 3.2 (1.4) | n.a |
| No. reflections | 581275 | 172532 | 303279 (13278) | n.a |
| No. Unique reflections | 79344 | 62713 | 93826 (9598) | 94155 (4843) |
| **Refinement** |  |  |  |  |
| $R_{work}$ (%) | 19.5 (24.7) |  |  |  |
| $R_{free}$ (%) | 24.5 (36.3) |  |  |  |
| No. reflections in FreeR set | 3979 (301) |  |  |  |
| No atoms | 11781 |  |  |  |
| Protein | 11421 |  |  |  |
| Ligands | 33 |  |  |  |
| Water | 327 |  |  |  |
| Average Bfactors (Å$^2$) |  |  |  |  |
| Protein | 28.2 |  |  |  |
| .....Ligands | 29.0 |  |  |  |
| Water | 23.6 |  |  |  |
| r.m.s deviations |  |  |  |  |
| Bond lengths (Å) | 0.012 |  |  |  |
| Bond angles (°) | 1.388 |  |  |  |
| Ramachandran |  |  |  |  |
| Most favoured (%) | 100 |  |  |  |
| Outliers (%) | 0 |  |  |  |

[a] Numbers in parentheses refer to the highest resolution shell. [b] processed using MOSFLM/SCALA. [c] processed using CrystalClear. [d] Scaling statistics not available due to back-up disc failure.