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Supporting information for article:

An unprecedented dioxygen species revealed by serial femtosecond rotational crystallography in copper nitrite reductase

Thomas P. Halsted, Keitaro Yamashita, Kunio Hirata, Hideo Ago, Go Ueno, Takehiko Tosha, Robert R. Eady, Svetlana V. Antonyuk, Masaki Yamamoto and S. Samar Hasnain

Supplementary information

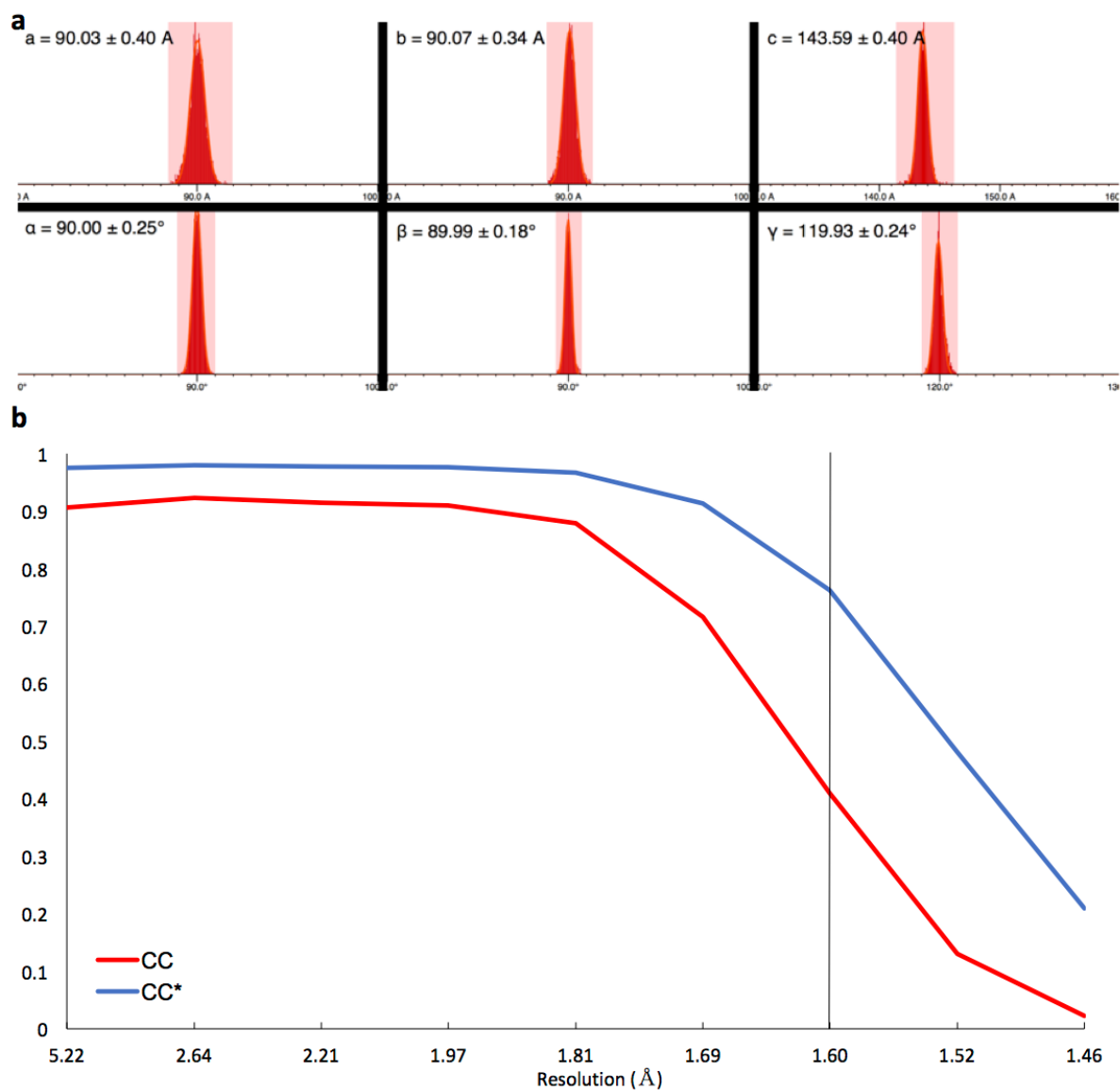


Figure S1 AxNiR SF-ROX data processing. **a.** The distribution of unit cell parameters displayed by *cell explorer*. The unit cell lengths and angles from individually indexed snapshots from *indexamajig* displayed as a distribution (White *et al.*, 2016). Red colouring represents these parameters that fall into a H centred space group. **b.** The correlation coefficient statistics for AxNiR, SF-ROX data processing. The CC and CC* vs the resolution during data processing. Data was cut-off at 1.6 \AA based on $CC_{1/2} = 0.5$. CC* is calculated from $CC_{1/2}$. $CC^* = [2 CC_{1/2}/(1 + CC_{1/2})]^{1/2}$ (Karplus & Diederichs, 2012).

AxNiR	1	-----DADKLPHTKVTLVAPPQVHPHEQATKSGPKVVEFTMTIEEKKMVI	45
AfNiR	1	MATAAEIAALPRQKVELVDPFVHAHSQVAEGGPKVVEFTMVEEKKIVI	50
AxNiR	46	DDKGTTLQAMTFNGSMPGPTLVVHEGDYVQLTLVNPATNAMPHNVDHGA	95
AfNiR	51	DDAGTEVHAMAFNGTVPGPLMVVHQDDYLELTLINPETNTLMHNIDFHAA	100
AxNiR	96	TGALGGAKLTNVNPGEQATLRFKADRSGETFVYHCAPEGMVPHVSVMSG	145
AfNiR	101	TGALGGGGLTEINPGEKTLRFKATKPGVFVYHCAPPGMVPHVSVGMNG	150
AxNiR	146	TLMVLPDRDGLKDPQGGKPLHYDRAYTIGEFDLIYIPKGPDKYKDYATLAES	195
AfNiR	151	AIMVLPREGLHDGKGGKALTYDKIYYVGEQDFYVPRDENGKYKYEAPGDA	200
AxNiR	196	YGDTVQVMRTLTPSHIVFNGKVGALTGANALTAKVGETVLLIHSQANRDT	245
AfNiR	201	YEDTVKVMRTLTPTHVVFNGAVGALTGDKAMTAAVGEKVLIVHSQANRDT	250
AxNiR	246	RPHLIGGHGDWVWETGKFANPPQRDLETWFIRGGSAGAALYTFKQPGVYA	295
AfNiR	251	RPHLIGGHGDYVWATGKFNTPDQETWFIPGGAAGAAFYTFQPGIYA	300
AxNiR	296	YLNHNLIIEAFELGAAGHIKVEGKWNDLDMKQIKAPAP--IPR	335
AfNiR	301	YVNHNLIEAFELGAAAHFKVTGEWDDLMTSVLAPSGTLVPR	342

Figure S2 AfNiR and AxNiR pairwise alignment. Compared using the EBLOSUM62 matrix. Similarity score of 77.5%.

References

- Karplus, P. A. & Diederichs, K. (2012). *Science* (80-.). **336**, 1030–1033.
- White, T. A., Mariani, V., Brehm, W., Yefanov, O., Barty, A., Beyerlein, K. R., Chervinskii, F., Galli, L., Gati, C., Nakane, T., Tolstikova, A., Yamashita, K., Yoon, C. H., Diederichs, K. & Chapman, H. N. (2016). *J. Appl. Crystallogr.* **49**, 680–689.