Table S1. Polymeric and NDUFA4 state in published mammalian complex IV structures, Related to Figure 6

Species	PDB ID	Method	Resolution (Å)	Polymeric State	NDUFA4 State	Reference
Bos taurus	1OCC	X-ray	2.8	dimer	missing	Tsukihara, T., Aoyama, H., Yamashita, E., Tomizaki, T., Yamaguchi, H., Shinzawa-Itoh, K., Nakashima, R., Yaono, R., Yoshikawa, S. (1996) The whole structure of the 13-subunit oxidized cytochrome c oxidase at 2.8 A.Science 272: 1136-1144
Bos taurus	1OCO	X-ray	2.8	dimer	missing	Yoshikawa, S., Shinzawa-Itoh, K., Nakashima, R., Yaono, R., Yamashita, E., Inoue, N., Yao, M., Fei, M.J., Libeu, C.P., Mizushima, T., Yamaguchi, H., Tomizaki, T., Tsukihara, T. (1998) Redox-coupled crystal structural changes in bovine heart cytochrome c oxidase. Science 280: 1723-1729
Bos taurus	1OCR	X-ray	2.35	dimer	missing	Yoshikawa, S., Shinzawa-Itoh, K., Nakashima, R., Yaono, R., Yamashita, E., Inoue, N., Yao, M., Fei, M.J., Libeu, C.P., Mizushima, T., Yamaguchi, H., Tomizaki, T., Tsukihara, T. (1998) Redox-coupled crystal structural changes in bovine heart cytochrome c oxidase. Science 280: 1723-1729
Bos taurus	1OCZ	X-ray	2.9	dimer	missing	Yoshikawa, S., Shinzawa-Itoh, K., Nakashima, R., Yaono, R., Yamashita, E., Inoue, N., Yao, M., Fei, M.J., Libeu, C.P., Mizushima, T., Yamaguchi, H., Tomizaki, T., Tsukihara, T. (1998) Redox-coupled crystal structural changes in bovine heart cytochrome c oxidase. Science 280: 1723-1729
Bos taurus	1V54	X-ray	1.8	dimer	missing	Tsukihara, T., Shimokata, K., Katayama, Y., Shimada, H., Muramoto, K., Aoyama, H., Mochizuki, M., Shinzawa-Itoh, K., Yamashita, E., Yao, M., Ishimura, Y., Yoshikawa, S. (2003) The low-spin heme of cytochrome c oxidase as the driving element of the proton-pumping process. Proc.Natl.Acad.Sci.Usa 100: 15304-15309
Bos taurus	1V55	X-ray	1.9	dimer	missing	Tsukihara, T., Shimokata, K., Katayama, Y., Shimada, H., Muramoto, K., Aoyama, H., Mochizuki, M., Shinzawa-Itoh, K., Yamashita, E., Yao, M., Ishimura, Y., Yoshikawa, S. (2003) The low-spin heme of cytochrome c oxidase as the driving element of the proton-pumping process. Proc.Natl.Acad.Sci.Usa 100: 15304-15309
Bos taurus	2DYR	X-ray	1.8	dimer	missing	Shinzawa-Itoh, K., Aoyama, H., Muramoto, K., Terada, H., Kurauchi, T., Tadehara, Y., Yamasaki, A., Sugimura, T., Kurono, S., Tsujimoto, K., Mizushima, T., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2007) Structures and physiological roles of 13 integral lipids of bovine heart cytochrome c oxidase. Embo J. 26: 1713-1725
Bos taurus	2DYS	X-ray	2.2	dimer	missing	Shinzawa-Itoh, K., Aoyama, H., Muramoto, K., Terada, H., Kurauchi, T., Tadehara, Y., Yamasaki, A., Sugimura, T., Kurono, S., Tsujimoto, K., Mizushima, T., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2007) Structures and physiological roles of 13 integral lipids of bovine heart cytochrome c oxidase. Embo J. 26: 1713-1725
Bos taurus	2EIJ	X-ray	1.9	dimer	missing	Muramoto, K., Hirata, K., Shinzawa-Itoh, K., Yoko-o, S., Yamashita, E., Aoyama, H., Tsukihara, T., Yoshikawa, S. (2007) A histidine residue acting as a controlling site for dioxygen reduction and proton pumping by cytochrome c oxidase. Proc.Natl.Acad.Sci.Usa 104: 7881-7886
Bos taurus	2EIK	X-ray	2.1	dimer	missing	Muramoto, K., Hirata, K., Shinzawa-Itoh, K., Yoko-o, S., Yamashita, E., Aoyama, H., Tsukihara, T., Yoshikawa, S. (2007) A histidine residue acting as a controlling site for dioxygen reduction and proton pumping by cytochrome c oxidase. Proc.Natl.Acad.Sci.Usa 104: 7881-7886
Bos taurus	2EIL	X-ray	2.1	dimer	missing	Muramoto, K., Hirata, K., Shinzawa-Itoh, K., Yoko-o, S., Yamashita, E., Aoyama, H., Tsukihara, T., Yoshikawa, S. (2007) A histidine residue acting as a controlling site for dioxygen reduction and proton pumping by cytochrome c oxidase. Proc.Natl.Acad.Sci.Usa 104: 7881-7886
Bos taurus	2EIM	X-ray	2.6	dimer	missing	Muramoto, K., Hirata, K., Shinzawa-Itoh, K., Yoko-o, S., Yamashita, E., Aoyama, H., Tsukihara, T., Yoshikawa, S. (2007) A histidine residue acting as a controlling site for dioxygen reduction and proton pumping by cytochrome c oxidase. Proc.Natl.Acad.Sci.Usa 104: 7881-7886
Bos taurus	2EIN	X-ray	2.7	dimer	missing	Muramoto, K., Hirata, K., Shinzawa-Itoh, K., Yoko-o, S., Yamashita, E., Aoyama, H., Tsukihara, T., Yoshikawa, S. (2007) A histidine residue acting as a controlling site for dioxygen reduction and proton pumping by cytochrome c oxidase. Proc.Natl.Acad.Sci.Usa 104: 7881-7886

Bos taurus	2OCC	X-ray	2.3	dimer	missing	Yoshikawa, S., Shinzawa-Itoh, K., Nakashima, R., Yaono, R., Yamashita, E., Inoue, N., Yao, M., Fei, M.J., Libeu, C.P., Mizushima, T., Yamaguchi, H., Tomizaki, T., Tsukihara, T (1998). Redox-coupled crystal structural changes in bovine heart cytochrome c oxidase. Science 280: 1723-1729
Bos taurus	2Y69	X-ray	1.95	dimer	missing	Kaila, V.R.I., Oksanen, E., Goldman, A., Bloch, D.A., Verkhovsky, M.I., Sundholm, D., Wikstrom, M. (2011) A Combined Quantum Chemical and Crystallographic Study on the Oxidized Binuclear Center of Cytochrome C Oxidase. Biochim.Biophys.Acta 1807: 769
Bos taurus	2ZXW	X-ray	2.5	dimer	missing	Aoyama, H., Muramoto, K., Shinzawa-Itoh, K., Hirata, K., Yamashita, E., Tsukihara, T., Ogura, T., Yoshikawa, S. (2009) A peroxide bridge between Fe and Cu ions in the O2 reduction site of fully oxidized cytochrome c oxidase could suppress the proton pump. Proc.Natl.Acad.Sci.USA 106: 2165-2169
Bos taurus	3ABK	X-ray	2.0	dimer	missing	Ohta, K., Muramoto, K., Shinzawa-Itoh, K., Yamashita, E., Yoshikawa, S., Tsukihara, T. (2010) X-ray structure of the NO-bound Cu(B) in bovine cytochrome c oxidase. Acta Crystallogr.,Sect.F 66: 251-253
Bos taurus	3ABL	X-ray	2.1	dimer	missing	Aoyama, H., Muramoto, K., Shinzawa-Itoh, K., Hirata, K., Yamashita, E., Tsukihara, T., Ogura, T., Yoshikawa, S. (2009) A peroxide bridge between Fe and Cu ions in the O2 reduction site of fully oxidized cytochrome c oxidase could suppress the proton pump. Proc.Natl.Acad.Sci.USA 106: 2165-2169
Bos taurus	3ABM	X-ray	1.95	dimer	missing	Aoyama, H., Muramoto, K., Shinzawa-Itoh, K., Hirata, K., Yamashita, E., Tsukihara, T., Ogura, T., Yoshikawa, S. (2009) A peroxide bridge between Fe and Cu ions in the O2 reduction site of fully oxidized cytochrome c oxidase could suppress the proton pump. Proc.Natl.Acad.Sci.USA 106: 2165-2169
Bos taurus	3AG1	X-ray	2.2	dimer	missing	Muramoto, K., Ohta, K., Shinzawa-Itoh, K., Kanda, K., Taniguchi, M., Nabekura, H., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2010) Bovine cytochrome c oxidase structures enable O2 reduction with minimization of reactive oxygens and provide a proton-pumping gate. Proc.Natl.Acad.Sci.USA 107: 7740-7745
Bos taurus	3AG2	X-ray	1.8	dimer	missing	Muramoto, K., Ohta, K., Shinzawa-Itoh, K., Kanda, K., Taniguchi, M., Nabekura, H., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2010) Bovine cytochrome c oxidase structures enable O2 reduction with minimization of reactive oxygens and provide a proton-pumping gate. Proc.Natl.Acad.Sci.USA 107: 7740-7745
Bos taurus	3AG3	X-ray	1.8	dimer	missing	Muramoto, K., Ohta, K., Shinzawa-Itoh, K., Kanda, K., Taniguchi, M., Nabekura, H., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2010) Bovine cytochrome c oxidase structures enable O2 reduction with minimization of reactive oxygens and provide a proton-pumping gate. Proc.Natl.Acad.Sci.USA 107: 7740-7745
Bos taurus	3AG4	X-ray	2.05	dimer	missing	Muramoto, K., Ohta, K., Shinzawa-Itoh, K., Kanda, K., Taniguchi, M., Nabekura, H., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2010) Bovine cytochrome c oxidase structures enable O2 reduction with minimization of reactive oxygens and provide a proton-pumping gate. Proc.Natl.Acad.Sci.USA 107: 7740-7745
Bos taurus	3ASN	X-ray	3.0	dimer	missing	Suga, M., Yano, N., Muramoto, K., Shinzawa-Itoh, K., Maeda, T., Yamashita, E., Tsukihara, T., Yoshikawa, S. Distinguishing between Cl- and O2(2-) as the bridging element between Fe3+ and Cu2+ in resting-oxidized cytochrome c oxidase. (2011) Acta Crystallogr.,Sect.D 67: 742-744
Bos taurus	3ASO	X-ray	2.3	dimer	missing	Suga, M., Yano, N., Muramoto, K., Shinzawa-Itoh, K., Maeda, T., Yamashita, E., Tsukihara, T., Yoshikawa, S. Distinguishing between Cl- and O2(2-) as the bridging element between Fe3+ and Cu2+ in resting-oxidized cytochrome c oxidase. (2011) Acta Crystallogr.,Sect.D 67: 742-744
Bos taurus	3WG7	X-ray	1.9	dimer	missing	Hirata, K., Shinzawa-Itoh, K., Yano, N., Takemura, S., Kato, K., Hatanaka, M., Muramoto, K., Kawahara, T., Tsukihara, T., Yamashita, E., Tono, K., Ueno, G., Hikima, T., Murakami, H., Inubushi, Y., Yabashi, M., Ishikawa, T., Yamamoto, M., Ogura, T., Sugimoto, H., Shen, J.R., Yoshikawa, S., Ago, H. (2014) Determination of damage-free crystal structure of an X-ray-sensitive protein using an XFEL. Nat.Methods Jul;11(7):734-6
Bos taurus	3X2Q	X-ray	2.0	dimer	missing	Yano, N., Muramoto, K., Mochizuki, M., Shinzawa-Itoh, K., Yamashita, E., Yoshikawa, S., Tsukihara, T. (2015) X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 A resolution. Acta Crystallogr.,Sect.F 71: 726-730

Bos taurus	5B1A	X-ray	1.5	dimer	missing	Yano, N., Muramoto, K., Shimada, A., Takemura, S., Baba, J., Fujisawa, H., Mochizuki, M., Shinzawa-Itoh, K., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2016) The Mg2+-containing Water Cluster of Mammalian Cytochrome c Oxidase Collects Four Pumping Proton Equivalents in Each Catalytic Cycle. J.Biol.Chem. 291: 23882-23894
Bos taurus	5B1B	X-ray	1.6	dimer	missing	Yano, N., Muramoto, K., Shimada, A., Takemura, S., Baba, J., Fujisawa, H., Mochizuki, M., Shinzawa-Itoh, K., Yamashita, E., Tsukihara, T., Yoshikawa, S. (2016) The Mg2+-containing Water Cluster of Mammalian Cytochrome c Oxidase Collects Four Pumping Proton Equivalents in Each Catalytic Cycle. J.Biol.Chem. 291: 23882-23894
Bos taurus	5B3S	X-ray	1.68	dimer	missing	Shimada, A., Baba, J., Yamashita, E., Shinzawa-Ito, K., Yoshikawa, S., Tsukihara, T. Bovine heart cytochrome c oxidase in the carbon monoxide-bound mixed-valence state at 1.68 angstrom resolution. (50 K)
Bos taurus	5IY5	X-ray	2.0	dimer	missing	Shimada, S., Shinzawa-Itoh, K., Baba, J., Aoe, S., Shimada, A., Yamashita, E., Kang, J., Tateno, M., Yoshikawa, S., Tsukihara, T. (2017) Complex structure of cytochrome c-cytochrome c oxidase reveals a novel protein-protein interaction mode EMBO J. 36: 291-300
Bos taurus	5W97	X-ray	2.3	dimer	missing	Ishigami, I., Zatsepin, N.A., Hikita, M., Conrad, C.E., Nelson, G., Coe, J.D., Basu, S., Grant, T.D., Seaberg, M.H., Sierra, R.G., Hunter, M.S., Fromme, P., Fromme, R., Yeh, S.R., Rousseau, D.L. (2017) Crystal structure of CO-bound cytochrome c oxidase determined by serial femtosecond X-ray crystallography at room temperature. Proc. Natl. Acad. Sci. U.S.A. 114: 8011-8016
Bos taurus	5WAU	X-ray	1.95	dimer	missing	Ishigami, I., Zatsepin, N.A., Hikita, M., Conrad, C.E., Nelson, G., Coe, J.D., Basu, S., Grant, T.D., Seaberg, M.H., Sierra, R.G., Hunter, M.S., Fromme, P., Fromme, R., Yeh, S.R., Rousseau, D.L. (2017) Crystal structure of CO-bound cytochrome c oxidase determined by serial femtosecond X-ray crystallography at room temperature. Proc. Natl. Acad. Sci. U.S.A. 114: 8011-8016
Bos taurus	5X19	X-ray	2.2	dimer	missing	Shimada, A., Kubo, M., Baba, S., Yamashita, K., Hirata, K., Ueno, G., Nomura, T., Kimura, T., Shinzawa-Itoh, K., Baba, J., Hatano, K., Eto, Y., Miyamoto, A., Murakami, H., Kumasaka, T., Owada, S., Tono, K., Yabashi, M., Yamaguchi, Y., Yanagisawa, S., Sakaguchi, M., Ogura, T., Komiya, R., Yan, J., Yamashita, E., Yamamoto, M., Ago, H., Yoshikawa, S., Tsukihara, T. (2017) A nanosecond time-resolved XFEL analysis of structural changes associated with CO release from cytochrome c oxidase. Sci Adv 3: e1603042-e1603042
Bos taurus	5X1B	X-ray	2.4	dimer	missing	Shimada, A., Kubo, M., Baba, S., Yamashita, K., Hirata, K., Ueno, G., Nomura, T., Kimura, T., Shinzawa-Itoh, K., Baba, J., Hatano, K., Eto, Y., Miyamoto, A., Murakami, H., Kumasaka, T., Owada, S., Tono, K., Yabashi, M., Yamaguchi, Y., Yanagisawa, S., Sakaguchi, M., Ogura, T., Komiya, R., Yan, J., Yamashita, E., Yamamoto, M., Ago, H., Yoshikawa, S., Tsukihara, T. (2017) A nanosecond time-resolved XFEL analysis of structural changes associated with CO release from cytochrome c oxidase. Sci Adv 3: e1603042-e1603042
Bos taurus	5X1F	X-ray	2.2	dimer	missing	Shimada, A., Kubo, M., Baba, S., Yamashita, K., Hirata, K., Ueno, G., Nomura, T., Kimura, T., Shinzawa-Itoh, K., Baba, J., Hatano, K., Eto, Y., Miyamoto, A., Murakami, H., Kumasaka, T., Owada, S., Tono, K., Yabashi, M., Yamaguchi, Y., Yanagisawa, S., Sakaguchi, M., Ogura, T., Komiya, R., Yan, J., Yamashita, E., Yamamoto, M., Ago, H., Yoshikawa, S., Tsukihara, T. (2017) A nanosecond time-resolved XFEL analysis of structural changes associated with CO release from cytochrome c oxidase. Sci Adv 3: e1603042-e1603042
Bos taurus	5XDQ	X-ray	1.77	dimer	missing	Luo, F.J., Shinzawa-Itoh, K., Hagimoto, N., Shimada, A., Shimada, S., Yamashita, E., Yoshikawa, S., Tsukihara, T. (2017) Structure of bovine cytochrome c oxidase crystallized at a neutral pH using a fluorinated detergent Acta Crystallogr.,Sect.F 73: 416-422
Bos taurus	5LUF	electron microscopy	9.1	monomer	missing	Sousa, J.S., Mills, D.J., Vonck, J., Kuhlbrandt, W. (2016) Functional asymmetry and electron flow in the bovine respirasome. Elife 2016 Nov 10;5
Sus scrofa	5GPN	electron microscopy	5.4	monomer	missing	Gu, J., Wu, M., Guo, R., Yan, K., Lei, J., Gao, N., Yang, M.(2016) The architecture of the mammalian respirasome. Nature 537: 639-64

Sus scrofa	5GUP	electron microscopy	4.0	monomer	missing	Wu, M., Gu, J., Guo, R., Huang, Y., Yang, M.(2016) Structure of Mammalian Respiratory Supercomplex I1III2IV1 Cell 167: 1598-1609.e10
Ovis aries	5J4Z	electron microscopy	5.8	monomer	missing	Letts, J.A., Fiedorczuk, K., Sazanov, L.A. (2016) The architecture of respiratory supercomplexes. Nature 537: 644-648
Ovis aries	5J7Y	electron microscopy	6.7	monomer	missing	Letts, J.A., Fiedorczuk, K., Sazanov, L.A. (2016) The architecture of respiratory supercomplexes. Nature 537: 644-648
Homo sapiens	5XTH	electron microscopy	3.9	monomer	missing	Guo, R., Zong, S., Wu, M., Gu, J., Yang, M. (2017) Architecture of Human Mitochondrial Respiratory Megacomplex I2III2IV2. Cell 170: 1247-1257.e12