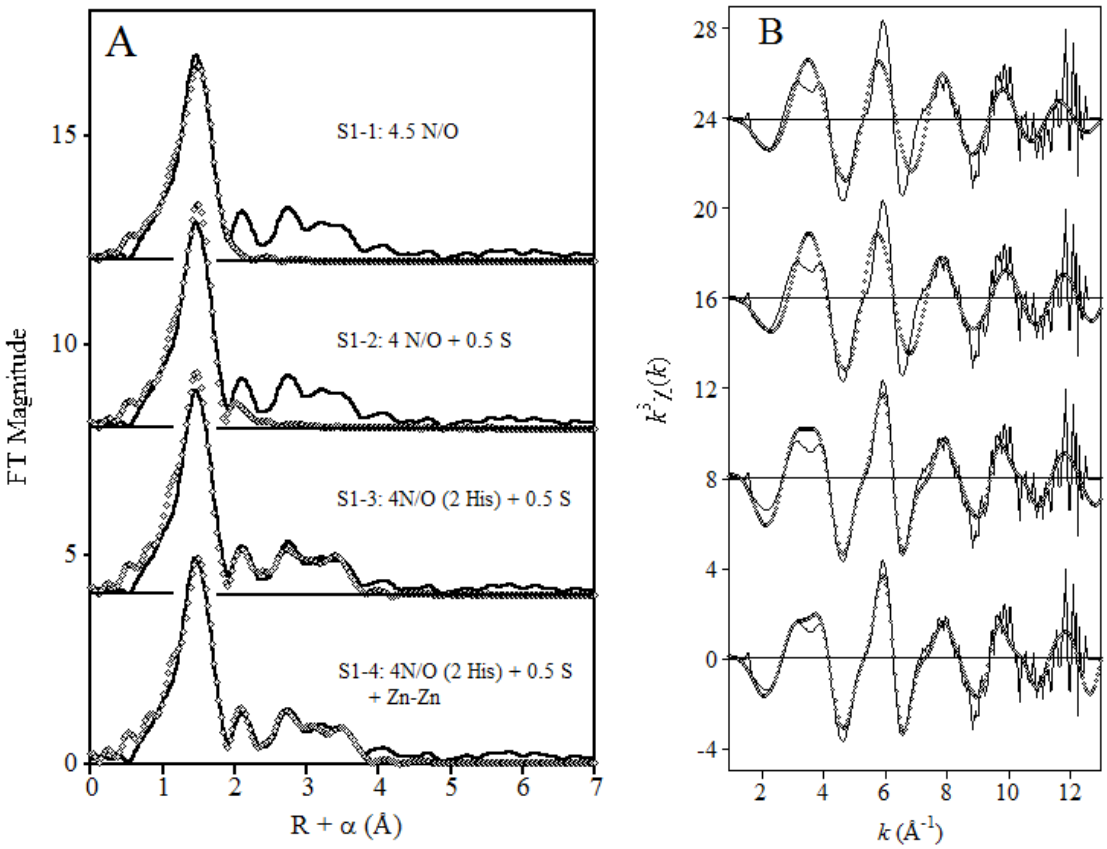

Figure S1. Fourier transforms (A) of k^3-weighted EXAFS (B) for 0.5Zn-BcII (solid lines), and corresponding curve fits (open symbols) from Table S1.

Table S1. Detailed EXAFS curve fitting results for 0.5Zn-BcII.[a]

Fit	Model	*Zn-N/O*	*Zn-S*	*Zn-His* [b]	*Zn-Zn*	R_f [c]	R_u [c]
S1-1	4.5 N/O	2.05 (6.6)				113	207
S1-2	4 N/O + 0.5 S	2.02 (4.9)	2.30 (5.8)			71	181
S1-3	4 N/O (2 His) + 0.5 S [d]	2.02 (4.5)	2.29 (6.3)	2.93 (0.6), 3.18 (2.0) 4.11 (10), 4.43 (14)		34	63
S1-4	4 N/O (3 His) + 0.5 S [e] + Zn-Zn	2.02 (5.0)	2.28 (8.0)	2.95 (1.6), 3.21 (5.0) 4.12 (9.0), 4.41 (21)	3.41 (13)	26	53
S1-5	4 N/O (3 His) + 0.5 S + 0.12 Zn-Zn [f]	2.02 (4.9)	2.28 (7.8)	2.94 (1.9), 3.21 (4.1) 4.12 (9.6), 4.41 (23)	3.41 (8.6)	28	57

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.5 Å^{-1}; R = 0.7-2.2 Å (fits 1-2) or 0.2-4.2 Å (fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as $1000 * \frac{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] - \left[\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2 \right] \right\}}{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] \right\}}$, where N is the number of data points.

[d] Inclusion of a Zn-C scattering path (0.5 C/Zn), along with the parameters of this fit, led to a refined Zn-C distance of 2.49 Å (σ^2 = 5.4 x 10^{-3} Å^2), with a modest decrease in fit residual to R_f = 25.

[e] Inclusion of a Zn-C scattering path (0.5 C/Zn), along with the parameters of this fit, led to a refined Zn-C distance of 2.50 Å (σ^2 = 5.1 x 10^{-3} Å^2), with a modest decrease in fit residual to R_f = 18.

[f] This fit allowed the Zn-Zn coordination number to float (refining to a value of 0.12), as well as R and σ^2.

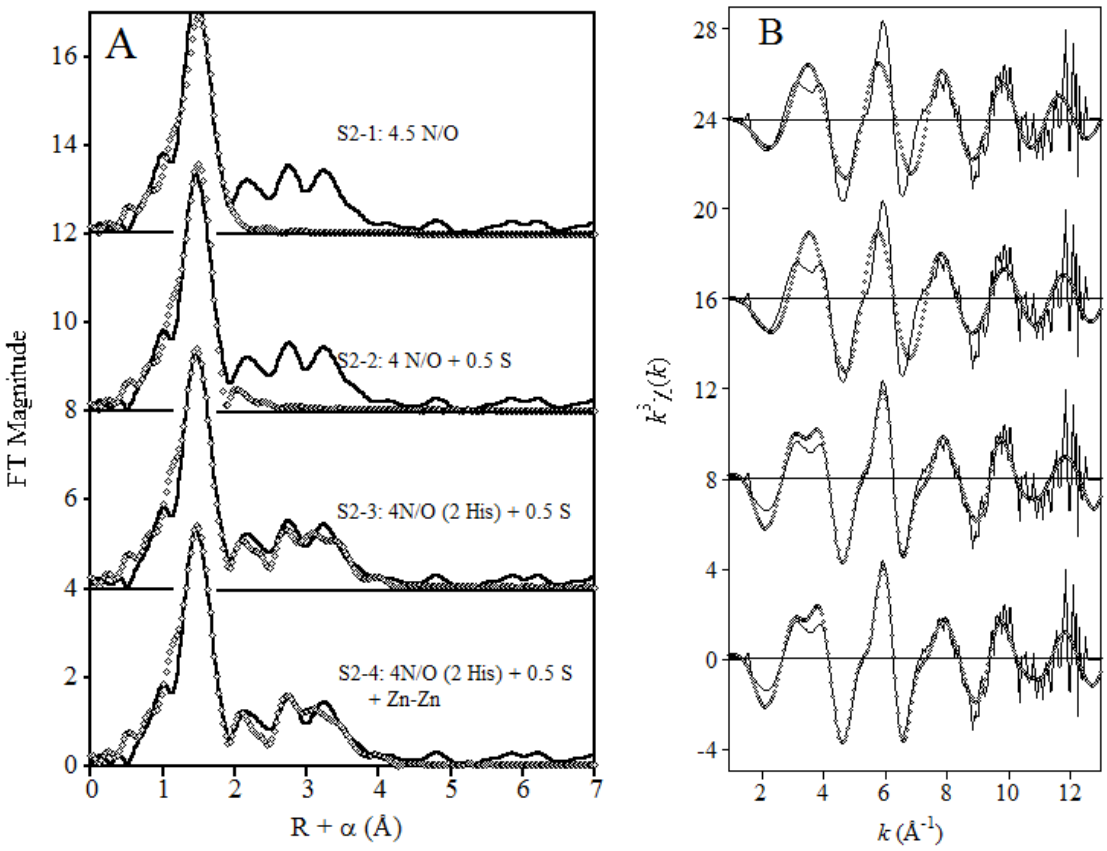

Figure S2. Fourier transforms (A) of k^3-weighted EXAFS (B) for 1Zn-BcII (solid lines), and corresponding curve fits (open symbols) from Table S5.

Table S2. Detailed EXAFS curve fitting results for 1Zn-BcII.[a]

Fit	Model	*Zn-N/O*	*Zn-S*	*Zn-His* [b]	*Zn-Zn*	R_f [c]	R_u [c]
S2-1	4.5 N/O	2.05 (4.6)				109	294
S2-2	4 N/O + 0.5 S	2.03 (5.0)	2.28 (6.3)			70	261
S2-3	4 N/O (2 His) + 0.5 S [d]	2.03 (4.5)	2.28 (6.3)	2.93 (0.6), 3.18 (2.0) 4.08 (12), 4.44 (14)		44	139
S2-4	4 N/O (3 His) + 0.5 S + Zn-Zn	2.03 (6.6)	2.28 (6.0)	2.93 (0.6), 3.18 (2.0) 4.08 (13), 4.44 (14)	3.41 (10)	31	46
S2-5	4 N/O (3 His) + 0.5 S + 0.30 Zn-Zn [e]	2.03 (6.7)	2.28 (6.3)	2.93 (0.4), 3.17 (1.5) 4.08 (12), 4.44 (13)	3.41 (8.7)	29	44

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.5 Å^{-1}; R = 0.7-2.2 Å (fits 1-2) or 0.2-4.2 Å (fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as

$$1000 * \frac{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] - \left[\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2 \right] \right\}}{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] \right\}},$$

where N is the number of data points.

[d] Inclusion of a Zn-C scattering path (0.5 C/Zn), along with the parameters of this fit, led to a refined Zn-C distance of 2.50 Å (σ^2 = 16 x 10^{-3} Å^2), with a modest decrease in fit residual to R_f = 39.

[e] This fit allowed the Zn-Zn coordination number to float (refining to a value of 0.30), as well as R and σ^2.

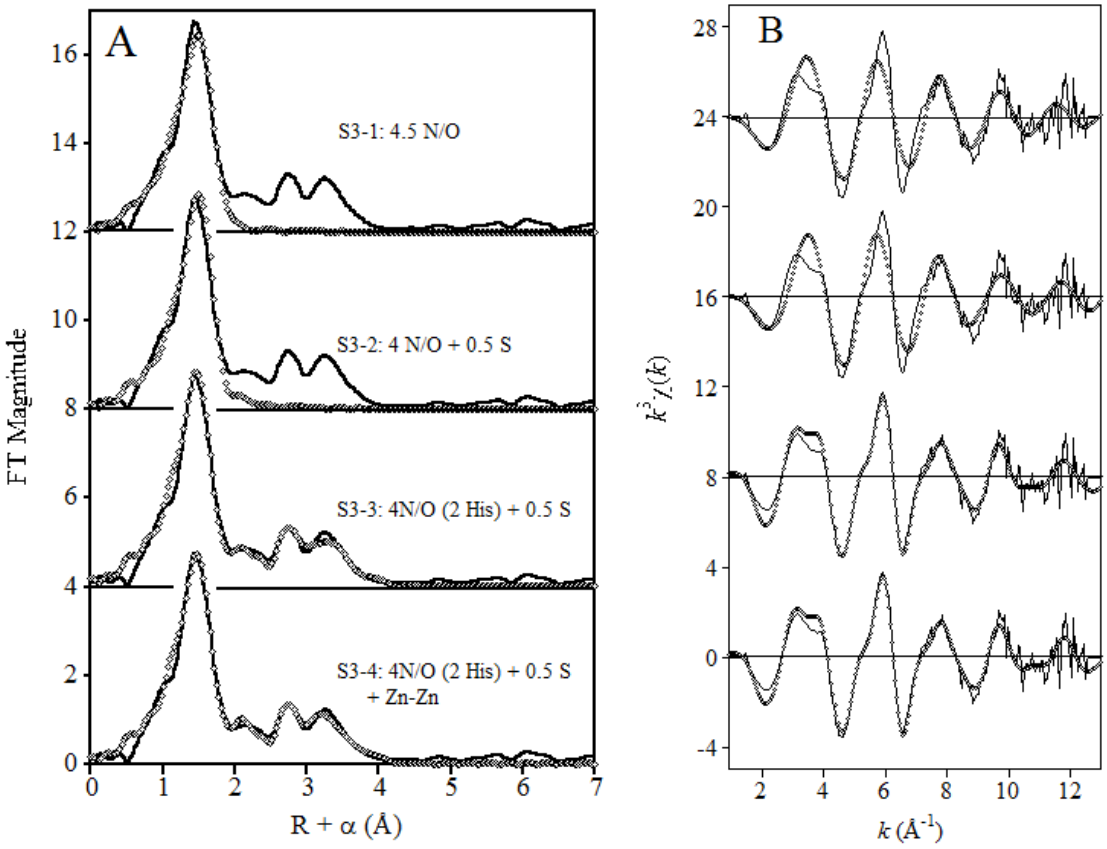

Figure S3. Fourier transforms (A) of k^3-weighted EXAFS (B) for 2Zn-BcII (solid lines), and corresponding curve fits (open symbols) from Table S6.

Table S3. Detailed EXAFS curve fitting results for 2Zn-BcII.[a]

Fit	Model	*Zn-N/O*	*Zn-S*	*Zn-His* [b]	*Zn-Zn*	R_f [c]	R_u [c]
S3-1	4.5 N/O	2.06 (6.4)				96	214
S3-2	4 N/O + 0.5 S	2.03 (5.9)	2.27 (6.4)			57	206
S3-3	4 N/O (2His) + 0.5 S [d]	2.03 (5.8)	2.27 (6.0)	2.93 (0.6), 3.17 (1.4) 4.09 (14), 4.43 (16)		19	89
S3-4	4 N/O (2His) + 0.5 S + Zn-Zn [e]	2.03 (6.3)	2.27 (2.6)	2.90 (3.1), 3.18 (5.8) 4.08 (11), 4.43 (15)	3.42 (8.3)	10	71
S3-5	4 N/O (2His) + 0.5 S + 0.91 Zn-Zn [f]	2.03 (6.0)	2.27 (2.5)	2.91 (3.0), 3.18 (5.7) 4.08 (11), 4.42 (16)	3.41 (8.0)	10	70

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.5 Å^{-1}; R = 0.7-2.3 Å (Fits 1-2) or 0.2-4.0 Å (Fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as

$$1000 * \frac{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] - \left[\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2 \right] \right\}}{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] \right\}},$$

where N is the number of data points.

[d] Addition of a Zn-C scattering path (0.5 C/Zn) to the parameters of this fit led to a refined Zn-C distance of 2.49 Å (σ^2 = 10 x 10^{-3} Å^2) and minimal improvement in fit residual to R_f = 16.

[e] Addition of a Zn-C scattering path (0.5 C/Zn) to the parameters of this fit led to a refined Zn-C distance of 2.50 Å (σ^2 = 1.3 x 10^{-3} Å^2) and minor improvement in fit residual to R_f = 9.

[f] This fit allowed the Zn-Zn coordination number to float (refining to a value of 0.91), as well as R and σ^2.

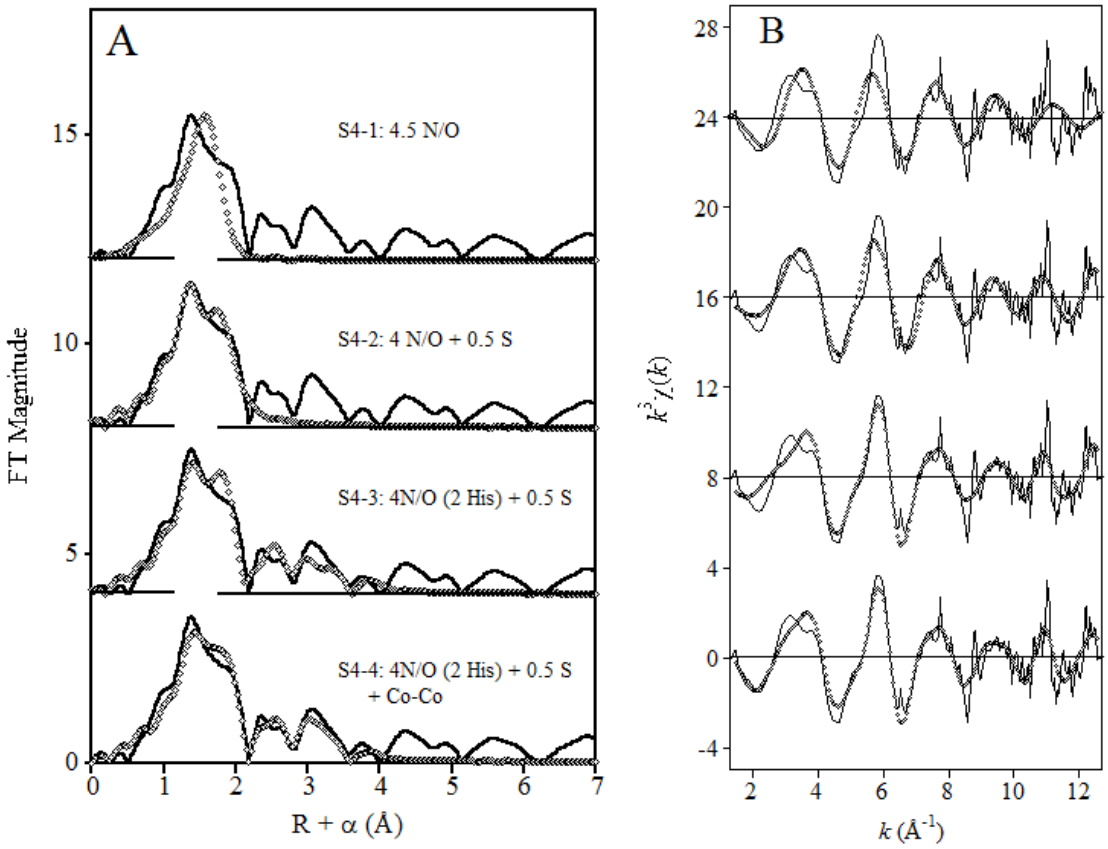

Figure S4. Fourier transforms (A) of k^3-weighted EXAFS (B) for 0.5Co-BcII (solid lines), and corresponding curve fits (open symbols) from Table S1.

Table S4. Detailed EXAFS curve fitting results for 0.5Co-BcII.[a]

Fit	Model	*Co-N/O*	*Co-S*	*Co-His* [b]	*Co-Co*	R_f [c]	R_u [c]
S4-1	4.5 N/O	2.10 (7.4)				152	384
S4-2	4 N/O + 0.5 S	2.02 (8.5)	2.30 (0.8)			32	255
S4-3	4 N/O (2His) + 0.5 S [d]	2.02 (8.4)	2.30 (0.9)	2.89 (4.2), 3.31 (20) 4.08 (6.4), 4.25 (9.5)		125	180
S4-4	4 N/O (2His) + 0.5 S + Co-Co [d]	2.03 (6.9)	2.30 (1.7)	2.94 (4.2), 3.25 (15) 4.03 (12), 4.28 (18)	3.56 (8.8)	76	134
S4-5	4 N/O (2His) + 0.5 S + 0.15 Co-Co [e]	2.03 (6.2)	2.30 (1.3)	2.93 (4.0), 3.26 (13) 4.03 (12), 4.29 (17)	3.56 (8.0)	83	144

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.5 Å^{-1}; R = 0.7-2.3 Å (fits 1-2) or 0.2-4.2 Å (fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as

$$1000 * \frac{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] - \left[\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2 \right] \right\}}{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] \right\}},$$

where N is the number of data points.

[d] Inclusion of a Co-C scattering path (0.5 C/Co), along with the parameters of this fit, led to a refined Co-C distance of 2.50 Å (σ^2 = 0.3 x 10^{-3} Å^2), with a modest decrease in fit residual to R_f = 113.

[e] This fit allowed the Co-Co coordination number to float (refining to a value of 0.15), as well as R and σ^2.

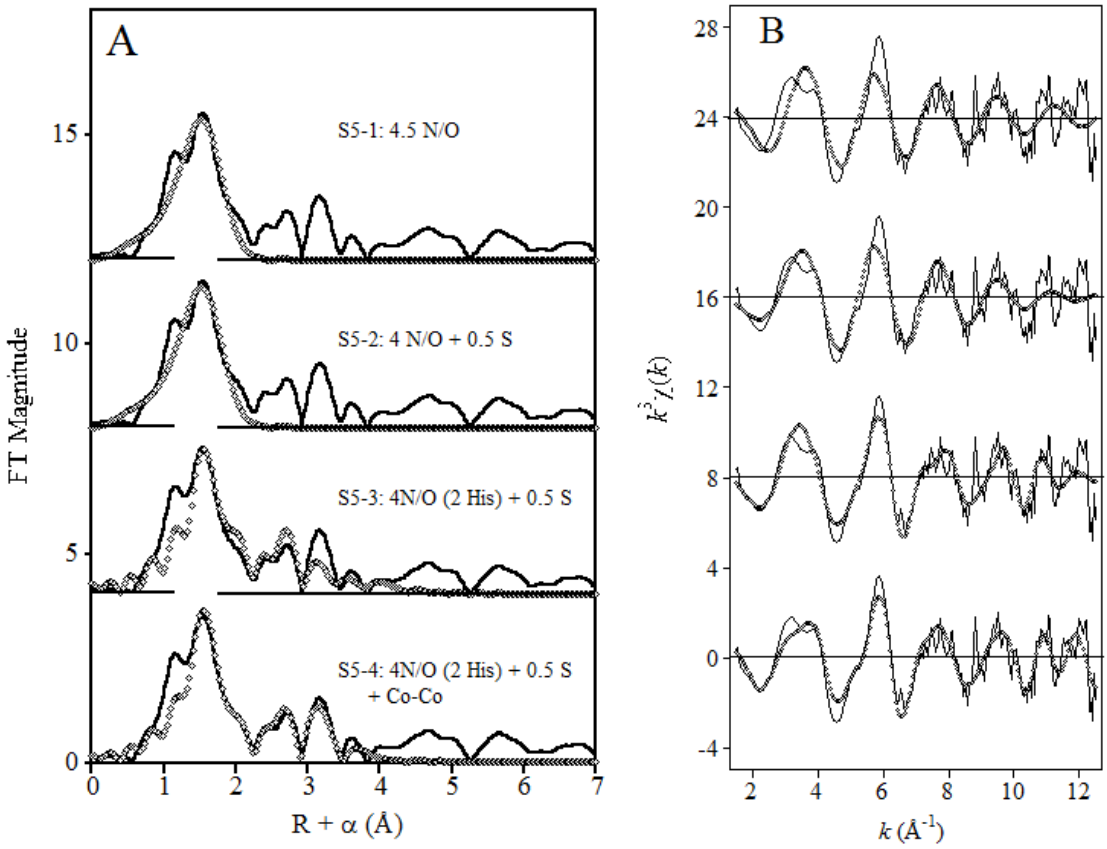

Figure S5. Fourier transforms (A) of k^3-weighted EXAFS (B) for 1Co-BcII (solid lines), and corresponding curve fits (open symbols) from Table S2.

Table S5. Detailed EXAFS curve fitting results for 1Co-BcII.[a]

Fit	Model	*Co-N/O*	*Co-S*	*Co-His* [b]	*Co-Co*	R_f [c]	R_u [c]
S5-1	4.5 N/O	2.11 (7.4)				124	384
S5-2	4 N/O + 0.5 S	2.03 (8.7)	2.30 (4.8)			47	355
S5-3	4 N/O (2His) + 0.5 S [d]	2.03 (7.7)	2.30 (5.0)	2.95 (2.0), 3.27 (20) 4.02 (23), 4.28 (13)		111	235
S5-4	4 N/O (2His) + 0.5 S + Co-Co [d]	2.03 (6.1)	2.30 (3.7)	2.94 (2.2), 3.25 (14) 4.02 (10), 4.28 (16)	3.55 (6.0)	63	177
S5-5	4 N/O (2His) + 0.5 S + 0.33 Co-Co [e]	2.02 (5.5)	2.30 (3.0)	2.94 (1.6), 3.27 (13) 4.02 (11), 4.28 (15)	3.55 (5.6)	60	170

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.5 Å^{-1}; R = 0.7-2.3 Å (fits 1-2) or 0.2-4.2 Å (fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as

$$1000 * \frac{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] - \left[\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2 \right] \right\}}{\sum_{i=1}^{N} \left\{ \left[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2 \right] \right\}}$$

, where N is the number of data points.

[d] Inclusion of a Co-C scattering path (0.5 C/Co), along with the parameters of this fit, led to a refined Co-C distance of 2.53 Å (σ^2 = 0.1 x 10^{-3} Å^2), with a modest decrease in fit residual to R_f = 100.

[e] This fit allowed the Co-Co coordination number to float (refining to a value of 0.33), as well as R and σ^2.

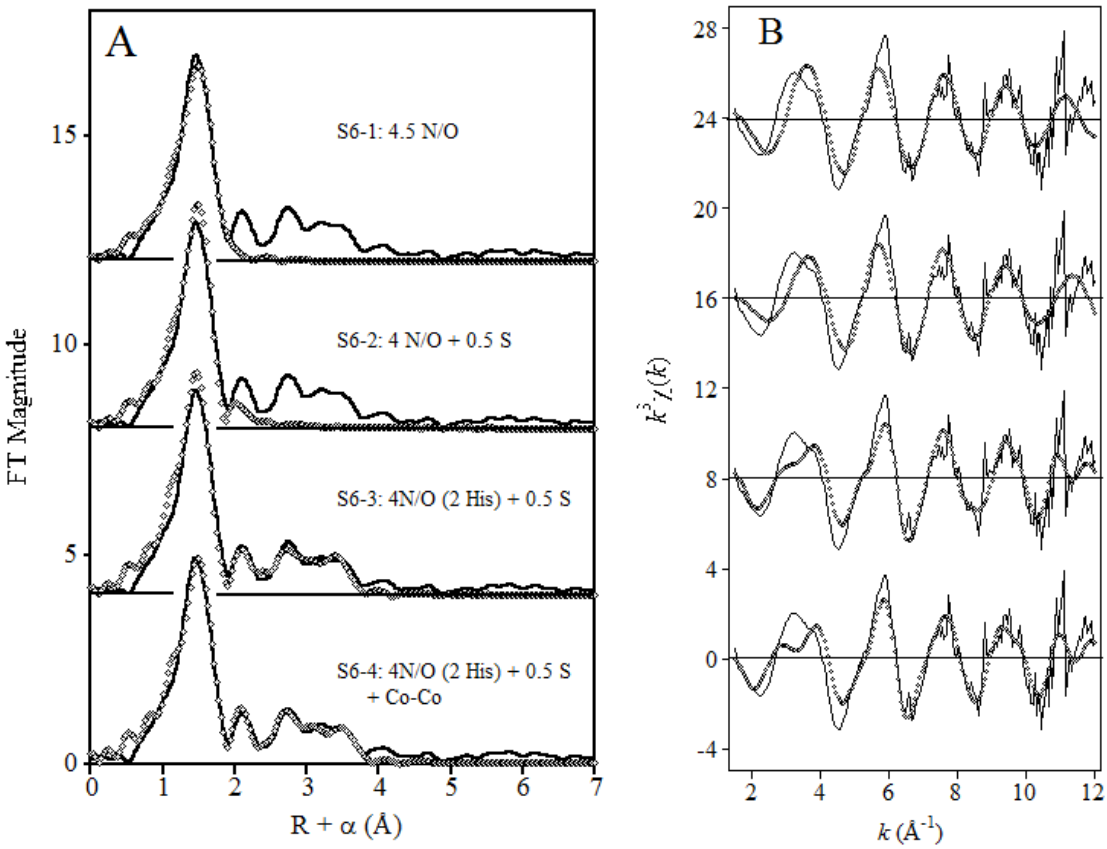

Figure S6. Fourier transforms (A) of k^3-weighted EXAFS (B) for CoCo-BcII (solid lines), and corresponding curve fits (open symbols) from Table S3.

Table S6. Detailed EXAFS curve fitting results for CoCo-BcII.[a]

Fit	Model	*Co-N/O*	*Co-S*	*Co-His* [b]	*Co-Co*	R_f [c]	R_u [c]
S6-1	4.5 N/O	2.14 (5.1)				119	309
S6-2	4 N/O + 0.5 S	2.09 (1.8)	2.31 (3.7)			92	288
S6-3	4 N/O (2His) + 0.5 S [d]	2.09 (2.6)	2.31 (1.5)	2.95 (5.8), 3.19 (16) 4.13 (6.9), 4.32 (6.6)		172	221
S6-4	4 N/O (2His) + 0.5 S + Co-Co [e]	2.09 (1.3)	2.31 (5.4)	2.93 (1.8), 3.19 (14) 4.08 (14), 4.32 (12)	3.55 (5.4)	125	202
S6-5	4 N/O (2His) + 0.5 S + 0.96 Co-Co [f]	2.09 (1.2)	2.31 (5.2)	2.93 (1.7), 3.19 (12) 4.08 (13), 4.31 (12)	3.55 (5.0)	120	198

[a] Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å^2)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [k = 1.5-12.4 Å^{-1}; R = 0.7-2.3 Å (fits 1-2) or 0.2-4.2 Å (fits 3-5)].

[b] Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

[c] Goodness of fit (R_f for fits to filtered data; R_u for fits to unfiltered data) defined as $1000 * \frac{\sum_{i=1}^{N} \{[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2] - [\mathrm{Re}(\chi_{i,calc})^2 + \mathrm{Im}(\chi_{i,calc})^2]\}}{\sum_{i=1}^{N} \{[\mathrm{Re}(\chi_{i,obs})^2 + \mathrm{Im}(\chi_{i,obs})^2]\}}$, where N is the number of data points.

[d] Addition of a Co-C scattering path (0.5 C/Co) to the parameters of this fit led to a refined Co-C distance of 2.47 Å (σ^2 = 1.9 x 10^{-3} Å^2), with a minimal decrease in fit residual to R_f = 168.

[e] Addition of a Co-C scattering path (0.5 C/Co) to the parameters of this fit led to a refined Co-C distance of 2.48 Å (σ^2 = 1.0 x 10^{-3} Å^2), with a minimal decrease in fit residual to R_f = 115.

[f] This fit allowed the Co-Co coordination number to float (refining to a value of 0.96), as well as R and σ^2.