The Effects of Select Histidine to Cysteine Mutations on Transcriptional Regulation by *E. coli* RcnR[‡]

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Supporting Information

Table S1 . Mutagenic Primers for RcnR Mutant Proteins with the Changes in Bold.

Mutant	Forward Primer	Reverse Primer
H60C	5'-CGGGAAGTGATTAAAGGT**TGT**CTGACGGAACACATCGTT -3'	5'-GAACGATGTGTTCCGTCAG**ACA**ACCTTTAATCACTTCCCG -3'
H64C	5'-GGTCATCTGACGGAA**TGC**ATCGTTCACCAGGGGG -3'	5'-CCCCCTGGTGAACGAT**GCA**TTCCGTCAGATGACC -3'
H67C	5'-GACGGAACACATCGTT**TGC**CAGGGGGATGAGC -3'	5'-GCTCATCCCCCTG**GCA**AACGATGTGTTCCGTC -3'

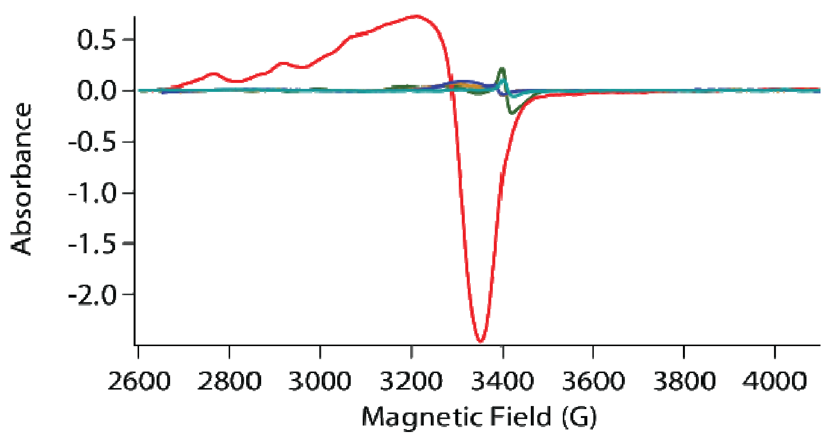

Figure S1. X-band EPR spectrum of Cu(I) H60C-RcnR in buffer with 300 mM NaBr (aqua), Cu(I) H64C-RcnR in buffer with 300mM NaBr(blue) and 300mM NaCl (orange), Cu(I) H67C-RcnR in buffer with 300 mM NaBr (green) and the Cu(II)-EDTA standard (red).

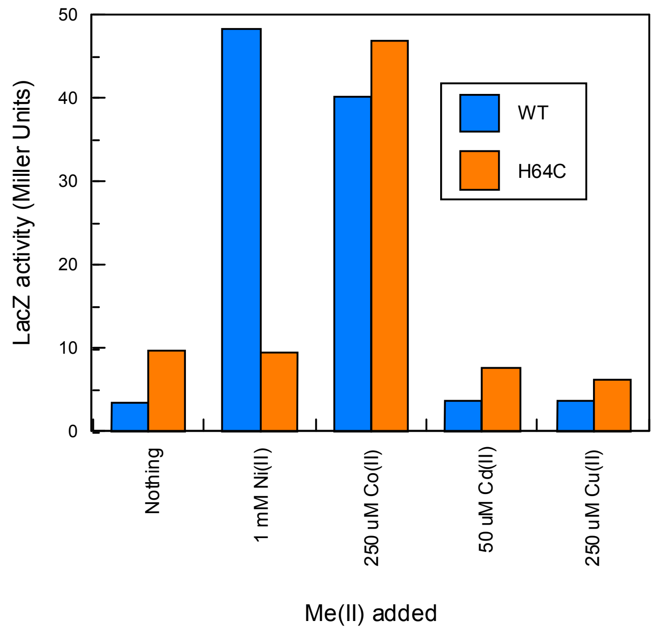

Figure S2. LacZ reporter assay showing the effects of the H64C-RcnR, mutation on the expression of P_{rcnA} expression response to Ni(II), Co(II), Cd(II) and Cu(II).

Table S2. XANES Analysis for the Metal Complexes of H60C-, H64C- and H67- RcnR Mutant Proteins in Buffer with 20 mM Hepes, with either 300 mM NaCl or 300 mM NaOAC (as noted) and 10 % Glycerol at pH 7.0. (In the case of the Cu(I) H64C-RcnR, the buffer also contained 2 mM TCEP).

Sample	1s→3d Peak area ($\times 10^{-2}$ eV)	1s→4pz Observed	Coordination Number	Edge Energy (eV)
		H60C		
Ni(II)[1]	3.2(7)	No	6	8342.9
		H64C		
Co(II)	6(1)	No	6	7720.8
Ni(II)	2.2(5)	Yes	4/5	8343.7
Cu(I)	NA	Yes	3	8987.7

[1]The sample was prepared in buffer with 300 mM NaOAc.

Additional fits for the XAS data are shown in the tables below. The best fits for the data are shown in bold and other acceptable fits are shown in italics.

Table S3. Additional Fits for Co(II) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_0 (eV)	R factor	χ^2	Reduced χ^2
5N/O	2.13(1)	1.1(8)	-13(3)	0.2145	396.04	23.57
5N/O	2.13(1)	1.1(8)				
1S	2.58(4)	6(5)	-12(3)	0.1756	324.28	21.91
5N/O	2.13(1)	1.0(8)				
1Im						
1S	2.61(4)	4(4)	0(3)	0.0873	161.29	23.72
5N/O	**2.13(1)**	**1.0(7)**				
2Im						
1S	**2.61(3)**	**4(3)**	**0(2)**	**0.0684**	**126.43**	**18.59**
5N/O	*2.13(1)*	*1.0(8)*				
3Im						
1S	*2.60(3)*	*4(4)*	*0(2)*	*0.0774*	*142.97*	*21.03*
2N/O	2.16(9)	2(4)				
3N/O	2.1(1)	0(11)				
1Im						
1S	2.59(5)	4(5)	-4(3)	0.0921	170.09	35.45
2N/O	2.16(8)	2(38)				
3N/O	2.2(1)	0(10)				
2Im						
1S	2.59(4)	3(4)	-4(3)	0.0755	139.45	29.06
3N/O	2.1(1)	0.6(230)				
2N/O	2.13(9)	0.8(374)				
1Im						
1S	2.61(5)	5(6)	-4(3)	0.0703	129.92	27.08
3N/O	2.1(1)	0.4(155)				
2N/O	2.14(6)	1(33)				
2Im						
1S	2.59(3)	3(4)	-3(2)	0.0667	123.17	25.67
4N/O	2.14(1)	0(0.9)				
1N/O	2.5(1)	4(18)				
1Im			2(3)	0.0639	118.11	24.61

1S	2.7(3)	18(48)				
1N/O	2.2(9)	14(233)				
4N/O	2.14(3)	0(2)				
1Im						
1S	2.6(3)	9(35)	-10(14)	0.1171	216.26	45.07

Table S4. Additional Fits for Ni(II) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
4N/O	2.07(2)	5(2)	-3(2)	0.2651	569.93	33.92
5N/O	2.07(2)	7(2)	-3(2)	0.2686	605.65	36.05
4N/O	2.09(1)	5(1)				
1S	2.65(1)	1(1)	0(1)	0.1078	243.23	16.43
5N/O	2.09(1)	7(1)				
1S	2.65(1)	2(1)	1(1)	0.1117	251.95	17.02
4N/O	2.07(2)	4(1)				
1S	2.56(7)	1(9)				
1Br	2.48(7)	4(4)	-1(2)	0.1137	256.47	20.04
5N/O	**2.080(7)**	**6.2(6)**				
1Im						
1S	**2.685(8)**	**1.0(7)**	**11(1)**	**0.0164**	**37.02**	**5.44**
5N/O	*2.079(7)*	*6.2(6)*				
2Im						
1S	*2.684(8)*	*0.9(7)*	*10.4(9)*	*0.0192*	*43.43*	*6.38*
5N/O	2.079(8)	6.2(7)				
3Im						
1S	2.684(9)	1.1(8)	10(1)	0.0215	48.39	7.16
2N/O	2.04(3)	4(5)				
3N/O	2.10(5)	9(6)				
1Im						
1S	2.68(5)	7(10)	2(2)	0.0345	74.17	15.45
3N/O	2.04(3)	7(4)				
2N/O	2.11(4)	5(4)				
1Im						
1S	2.69(6)	3(9)	3(2)	0.0263	59.37	12.37
4N/O	2.04(3)	7(2)				
1N/O	2.13(4)	1(4)				
1Im						
1S	2.69(9	0.6(72)	5(3)	0.0227	51.23	10.67

1N/O	2.04(3)	0(3)				
4N/O	2.10(8)	11(4)				
1Im						
1S	2.65(3)	2(2)	0(7)	0.0476	107.49	22.40

Table S5. Additional Fits for Ni(II) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaOAc and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
4N/O	2.07(1)	2(1)	-5(2)	0.1848	725.53	43.19
5N/O	2.07(1)	4(1)	-5(2)	0.1681	659.78	39.27
6N/O	2.07(1)	6(1)	-6(2)	0.1761	691.27	41.15
4N/O	2.08(1)	3(1)				
1S	2.60(2)	5(2)	-3(2)	0.1143	448.57	30.31
5N/O	2.08(1)	4.3(8)				
1S	2.60(2)	4(2)	-3(1)	0.0953	374.09	25.28
6N/O	2.08(1)	5.7(9)				
1S	2.59(2)	4(2)	-4(1)	0.1008	395.90	26.75
5N/O	2.072(7)	3.9(5)				
1Im						
1S	2.64(1)	3(1)	8(1)	0.0207	81.29	11.95
5N/O	2.073(7)	3.9(6)				
2Im						
1S	2.63(2)	4(2)	8(1)	0.0234	83.27	12.24
5N/O	2,073(8)	3.9(6)				
3Im						
1S	2.64(4)	4(2)	8(1)	0.0263	103.21	15.18
2N/O	2.01(2)	0.9(16)				
3N/O	2.13(2)	4(2)				
1Im						
1S	2.60(1)	3(3)	1(2)	0.0160	62.92	13.11
2N/O	2.01(2)	0.6(14)				
3N/O	2.14(2)	4(2)				
2Im						
1S	2.60(2)	3(2)	1(2)	0.0174	68.61	14.30
3N/O	*2.03(1)*	*2(1)*	*3(1)*	*0.0119*	*46.85*	*9.76*

2N/O	*2.16(2)*	*2(2)*				
1Im						
1S	*2.61(1)*	*3(2)*				
3N/O	*2.03(1)*	*2(1)*				
2N/O	*2.16(2)*	*2(2)*				
2Im						
1S	*2.61(1)*	*3(2)*	*3(2)*	*0.0139*	*54.78*	*11.41*
4N/O	**2.043(9)**	**2.5(8)**				
1N/O	**2.18(2)**	**0(3)**				
1Im						
1S	**2.62(1)**	**3(2)**	**5(1)**	**0.0104**	**41.13**	**8.57**
4N/O	*2.04(1)*	*2.6(9)*				
1N/O	*2.18(2)*	*0(3)*				
2Im						
1S	*2.62(2)*	*4(2)*	*5(1)*	*0.0126*	*49.75*	*10.37*
1N/O	2.02(8)	3(11)				
4N/O	2.09(4)	4(4)				
1Im						
1S	2.59(3)	4(4)	-2(3)	0.0364	142.85	29.77

Table S6. Additional Fits for Cu(I) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 $Å^{-1}$ and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} $Å^2$)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
1N/O	2.17(4)	0(4)	9.2(2)	0.5387	2742.05	163.23
2N/O	2.17(1)	0(1)	9.2(1)	0.3094	1574.95	93.75
1N/O	2.14(3)	1(4)				
2S	2.31(2)	5(1)	4(2)	0.0801	408.12	27.58
2N/O	2.19(5)	11(13)				
2S	2.30(1)	4(1)	4(2)	0.0852	433.88	29.32
1N/O	2.00(8)	6(6)				
1S	2.26(3)	0(1)				
1Br	2.47(3)	6(2)	-4(5)	0.0721	357.38	28.70
2N/O	2.08(9)	14(6)				
1S	2.28(2)	0(0.8)				
1Br	2.50(3)	8(2)	0(5)	0.0606	308.94	24.14
1N/O	2.14(3)	0.4(31)				
1Im						
2S	2.32(2)	5(2)	4(2)	0.0503	256.02	37.66
1N/O	2.09(5)	0(5)				
1Im						
1S	2.30(7)	2(3)				
1Br	2.50(3)	7(5)	2(6)	0.0491	92.08	19.19
2N/O	2.2(1)	20(24)				
1Im						
2S	2.30(2)	4(1)	2(5)	0.0552	280.98	41.33
2N/O	2.20(4)	6(16)				
2Im						
2S	2.31(2)	5(4)	5(2)	0.0594	302.37	44.48
2N/O	**2.13(2)**	**2(2)**				
1Im						
1S	**2.33(9)**	**7(6)**	**5(2)**	**0.0256**	**47.99**	**10.00**

1Br	**2.50(3)**	**7(2)**				
2N/O	*2.13(2)*	*1(2)*				
2Im						
1S	*2.36(7)*	*8(7)*				
1Br	*2.49(2)*	*7(3)*	*6(2)*	*0.0257*	*48.23*	*10.05*

Table S7. Additional Fits for Zn(II) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 $Å^{-1}$ and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 ($x10^{-3}$ $Å^2$)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
3N/O	2.15(1)	0(1)	-3(3)	0.2486	1004.49	59.79
4N/O	2.15(1)	2(1)	-4(3)	0.2587	1102.61	65.64
5N/O	2.14(2)	3(1)	-5(3)	0.2908	1239.42	73.78
5N/O 1S	2.27(5) 2.28(2)	18(9) 0(1)	-1(4)	0.2037	822.93	55.61
3N/O 2S	2.2(1) 2.23(7)	0(5) 1(5)	-8(7)	0.2070	882.12	59.61
4N/O 2S	2.24(6) 2.24(6)	0(10) 0(6)	-4(5)	0.1900	309.80	54.72
3N/O 2S 1Br	2.09(7) 2.3(1) 2.3(1)	5(7) 0(8) 2(4)	-11(6)	0.1665	709.57	55.44
5N/O 1Im 1S	2.18(3) 2.28(4)	4(4) 2(3)	7(4)	0.1021	435.14	64.01
5N/O 2Im 1S	2.11(4) 2.29(2)	11(4) 0(1)	-2(5)	0.0844	359.68	52.91
3N/O 1Im 2S 1Br	2.00(3) 2.36(3) 2.33(3)	7(3) 1(3) 0.2(15)	-9(3)	0.0265	113.11	23.57
3N/O **2Im** **2S** **1Br**	**2.00(3)** **2.36(3)** **2.33(3)**	**8(2)** **1(3)** **0.2(13)**	**-9(3)**	**0.0201**	**86.01**	**17.92**
3N/O	*2.00(4)*	*8(3)*	*-10(4)*	*0.0210*	*89.78*	*18.71*

3Im		
2S	*2.35(3)*	*0.3(29)*
1Br	*2.32(3)*	*0.1(15)*

Table S8. Additional Fits for Zn(II) H60C-RcnR in Buffer with 20 mM Hepes, 300 mM NaOAc and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^{-2})	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
2N/O	2.16(2)	0(1)	0(4)	0.3053	1593.63	94.87
3N/O	2.15(1)	2(1)	-1(3)	0.2095	1093.56	65.10
2N/O	2.04(3)	4(2)				
2S	2.28(1)	3.8(9)	-14(2)	0.0547	285.80	19.31
3N/O	2.07(2)	4(1)				
1S	2.30(1)	0.7(9)	-19(2)	0.0542	248.04	16.76
3N/O	2.08(5)	10(3)				
2S	2.28(1)	5(1)	-12(3)	0.0600	313.19	21.16
2N/O	2.02(1)	3.8(8)				
1Im						
2S	2.293(7)	3.9(4)	-9(1)	0.0081	42.35	6.22
2N/O	2.02(1)	3.8(8)				
2Im						
2S	2.293(7)	3.8(4)	-9(1)	0.0076	39.76	5.84
3N/O	2.07(1)	3.3(8)				
1Im						
1S	2.33(1)	1.0(6)	-2(2)	0.0176	92.12	13.55
3N/O	2.07(1)	3.4(8)				
2Im						
1S	2.32(1)	0.8(6)	-3(2)	0.0174	91.23	13.42
3N/O	2.07(1)	3.4(8)				
3Im						
1S	2.32(1)	0.8(6)	-3(2)	0.0175	91.55	13.46
3N/O	**2.04(1)**	**6.8(7)**				
1Im						
2S	**2.297(6)**	**4.5(3)**	**-8(1)**	**0.0051**	**26.90**	**3.95**
3N/O	*2.04(1)*	*6.7(8)*	*-8(1)*	*0.0053*	*27.70*	*4.07*

2Im						
2S	*2.299(7)*	*4.5(4)*				
3N/O	2.04(1)	6.7(8)				
3Im						
2S	2.299(8)	4.5(4)	-8(1)	0.0058	30.34	4.46

Table S9. Additional Fits for Co(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
3N/O	2.10(2)	5(1)	-9(2)	0.1631	340.11	20.24
4N/O	2.09(1)	7(1)	-10(2)	0.1138	237.26	14.12
5N/O	2.09(1)	9(1)	-11(2)	0.103	214.69	12.78
5N/O	2.10(3)	11(6)				
1S	2.22(6)	11(10)	-13(3)	0.0957	199.55	13.48
3N/O	2.05(4)	9(3)				
2S	2.25(3)	12(4)	-18(4)	0.1069	222.97	15.06
4N/O	2.12(2)	11(3)				
1S	1.86(3)	18(5)				
1Br	2.42(3)	15(4)	-5(2)	0.0694	144.82	11.31
3N/O	2.05(2)	6(2)				
2S	2.39(4)	13(5)				
1Br	2.38(3)	8(2)	-13(2)	0.0666	138.82	10.84
5N/O	2.05(2)	10(1)				
1Im						
1S	2.31(2)	8(2)	-6(2)	0.0277	57.74	8.49
5N/O	2.04(2)	11(1)				
2Im						
1S	2.29(2)	7(2)	-7(3)	0.0229	47.84	7.03
5N/O	2.05(3)	11(2)				
3Im						
1S	2.29(3)	7(2)	-8(4)	0.0249	51.94	7.64
3N/O	2.02(2)	6(2)				
1Im						
2S	2.33(4)	10(2)				
1Br	2.68(4)	7(3)	-9(4)	0.0368	76.74	15.99
3N/O	2.02(2)	6(1)	-8(3)	0.0138	28.76	5.99

2Im						
2S	2.33(3)	9(2)				
1Br	2.67(3)	6(2)				
3N/O	**2.03(2)**	**6(1)**				
3Im						
2S	**2.33(3)**	**9(1)**				
1Br	**2.67(3)**	**6(2)**	**-8(3)**	**0.0127**	**26.63**	**5.55**

Table S10. Additional Fits for Co(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
3N/O	2.16(2)	2(2)	-8(4)	0.3239	932.84	55.53
5N/O	2.15(2)	6(1)	-9(3)	0.2423	752.40	44.79
5N/O	2.0(6)	10(4)				
1S	2.28(3)	2(2)	-21(6)	0.2475	712.85	48.15
3N/O	1.97(5)	6(4)				
2S	2.25(3)	4(2)	-28(6)	0.2628	816.10	55.15
3N/O	2.07(5)	6(4)				
2S	2.32(4)	5(3)				
1Cl	2.53(4)	2(3)	-16(4)	0.1847	573.66	44.82
3N/O	2.03(4)	5(3)				
1Im						
2S	2.33(4)	2(2)				
1Cl	2.52(5)	0(3)	-11(5)	0.0789	245.13	51.09
3N/O	2.03(3)	5(2)				
2Im						
2S	2.34(3)	2(1)				
1Cl	2.52(3)	0(2)	-11(4)	0.0365	113.40	23.63
3N/O	**2.03(2)**	**5(1)**				
3Im						
2S	**2.34(2)**	**2(1)**				
1Cl	**2.51(2)**	**0(2)**	**-10(2)**	**0.0216**	**62.47**	**13.02**
5N/O	2.01(7)	9(4)				
1Im						
1S	2.29(4)	1(2)	-17(10)	0.2096	650.85	97.74

Table S11. Additional Fits for Ni(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
2N/O	2.09(2)	0(1)	0(3)	0.2477	345.26	20.55
3N/O	2.09(1)	1.9(9)	0(2)	0.1629	277.02	13.51
4N/O	2.09(1)	3.7(9)	-1(2)	0.1437	200.35	11.92
3N/O	2.08(4)	5(3)				
1S	2.24(3)	5(4)	-5(3)	0.1343	187.24	12.65
2N/O	2.04(3)	1(2)				
1S	2.26(2)	2(2)	-6(3)	0.1435	169.36	11.44
4N/O	2.11(3)	6(9)				
1S	2.21(7)	5(10)	-2(3)	0.1271	177.12	11.96
3N/O	2.07(3)	5(2)				
1S	2.24(3)	5(3)				
1Br	2.77(3)	10(3)	-5(3)	0.0884	123.29	9.63
2N/O	2.04(3)	2(2)				
1S	2.26(2)	2(2)				
1Br	2.76(3)	10(3)	-7(3)	0.0997	138.94	10.85
3N/O	2.04(1)	3(1)				
1Im						
1S	2.4(1)	28(28)	1(3)	0.0822	461.75	67.92
3N/O	2.04(1)	4(1)				
2Im						
1S	2.28(5)	14(8)	-1(3)	0.0555	311.94	45.88
3N/O	2.03(2)	4(1)				
3Im						
1S	2.28(2)	3(1)	1(2)	0.0425	59.26	8.71
3N/O	2.03(3)	4(3)				
1Im						
1S	2.28(5)	3(6)				
1Br	2.6(4)	18(37)	1(5)	0.0831	115.82	24.14

3N/O	2.06(1)	3(1)				
2Im						
1S	2.33(3)	5(3)				
1Br	2.71(3)	5(4)	6(2)	0.0299	41.73	8.69
3N/O	**2.05(1)**	**3(1)**				
3Im						
1S	**2.31(3)**	**4(3)**				
1Br	**2.69(5)**	**8(9)**	**5(2)**	**0.0263**	**36.78**	**7.66**
2N/O	2.00(6)	3(6)				
1Im						
1S	2.26(9)	0.1(4)				
1Br	2.5(2)	7(13)	-3(11)	0.1102	153.68	32.03
2N/O	*2.00(3)*	*3(3)*				
2Im						
1S	*2.25(4)*	*0(2)*				
1Br	*2.51(8)*	*6(6)*	*-3(4)*	*0.0442*	*61.68*	*12.85*

Table S12. Additional Fits for Ni(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
2N/O	2.07(2)	2(2)	0(3)	0.2892	2097.05	124.84
3N/O	2.07(2)	5(1)	0(2)	0.2195	1752.09	104.30
4N/O	2.06(2)	7(2)	-1(2)	0.2174	1735.48	103.31
2N/O	2.02(4)	4(3)				
1S	2.25(4)	6(4)	-5(4)	0.2142	1553.37	104.97
2N/O	2.04(5)	7(7)				
2S	2.21(4)	12(6)	-8(5)	0.2194	1750.88	118.32
3N/O	2.06(4)	8(6)				
1S	2.22(5)	10(10)	-3(3)	0.2040	1628.07	110.02
4N/O	2.10(5)	1(15)				
1S	2.2(1)	8(11)	-2(3)	0.1973	1574.96	106.43
3N/O	2.07(4)	7(6)				
2S	2.19(4)	15(11)	-6(3)	0.2103	1678.85	113.45
2N/O	2.04(2)	3(2)				
1S	2.31(4)	8(5)				
1Cl	2.61(3)	7(4)	-1(2)	0.1312	951.20	74.32
3N/O	2.07(2)	5(1)				
1S	2.4(1)	21(16)				
1Cl	2.63(3)	6(2)	0(2)	0.1103	880.51	68.80
2N/O	2.02(2)	2(1)				
1Im						
1S	2.32(3)	4(2)				
1Cl	2.57(5)	8(6)	6(2)	0.0557	444.89	92.72
2N/O	*2.01(2)*	*3(2)*				
2Im						
1S	*2.30(3)*	*4(2)*				
1Cl	*2.52(7)*	*11(9)*	*5(2)*	*0.0502*	*401.22*	*83.62*

3N/O	**2.03(2)**	**5(1)**				
1Im						
1S	**2.34(4)**	**8(4)**				
1Cl	**2.61(4)**	**7(5)**	**8(3)**	**0.0441**	**352.90**	**73.47**
3N/O	*2.03(2)*	*6(2)*				
2Im						
1S	*2.32(5)*	*7(3)*				
1Cl	*2.58(7)*	*11(12)*	*7(3)*	*0.0462*	*369.21*	*76.95*
3N/O	*2.03(2)*	*6(3)*				
3Im						
1S	*2.29(6)*	*7(4)*				
1Cl	*2.5(2)*	*20(34)*	*5(3)*	*0.0497*	*396.91*	*82.72*

Table S13. Additional Fits for Cu(I) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^{-2})	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
1N/O	2.16(4)	0(4)	9(6)	0.5532	1035.93	61.67
2N/O	2.16(2)	0.7(17)	9(2)	0.3685	690.15	41.08
2N/O	2.11(1)	0(1)				
1S	2.36(1)	0.6(12)	5(1)	0.1056	197.82	13.36
1N/O	2.09(2)	0(2)				
2S	2.34(1)	5(1)	3(2)	0.0918	146.59	9.90
2N/O	2.12(2)	3(2)				
1S	2.32(3)	4(3)				
1Br	2.51(2)	7(2)	4(2)	0.0564	105.64	8.25
1N/O	2.11(2)	0.1(22)				
2S	2.31(4)	9(2)				
1Br	2.49(2)	7(2)	1(3)	0.0490	91.91	7.18
2N/O	2.11(2)	0(2)				
1Im						
1S	2.36(2)	0.7(15)	6(2)	0.0701	131.37	19.32
2N/O	2.11(1)	0(1)				
2Im						
1S	2.37(2)	0.7(1)	6(2)	0.0514	96.32	14.17
2N/O	**2.12(2)**	**2(3)**				
1Im						
1S	**2.32(6)**	**6(5)**				
1Br	**2.50(2)**	**7(2)**	**4(2)**	**0.0218**	**40.84**	**8.51**
2N/O	2.13(2)	1(2)				
2Im						
1S	2.36(7)	8(7)				
1Br	2.49(2)	7(3)	6(2)	0.0257	48.23	10.05
1N/O	2.11(3)	0(3)				
1Im			2(4)	0.0292	46.63	9.72

2S	2.32(6)	9(3)
1Br	2.48(2)	8(3)

Table S14. Additional Fits for Cu(I) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaCl and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
1N/O	2.14(3)	0(3)	8(5)	0.4422	878.37	52.29
2N/O	2.14(1)	0(1)	7(2)	0.2115	364.37	21.69
2N/O	2.12(2)	3(2)				
1S	2.31(2)	4(2)	4(1)	0.0632	125.73	8.49
1N/O	2.11(2)	2(3)				
2S	2.29(2)	7(1)	0(2)	0.0586	116.44	7.86
2N/O	2.10(1)	0.8(9)				
1Im						
1S	2.36(2)	3(1)	12(2)	0.0351	69.83	10.27
2N/O	**2.10(1)**	**0.9(9)**				
2Im						
1S	**2.36(2)**	**3(1)**	**12(2)**	**0.0340**	**67.71**	**9.96**
1N/O	2.07(3)	2(3)				
1Im						
2S	2.30(2)	6(1)	2(4)	0.0443	88.01	12.94

Table S15. Additional Fits for Zn(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
3N/O	2.15(2)	2(1)	-5(3)	0.2818	697.29	41.51
4N/O	2.14(2)	4(1)	-6(3)	0.2265	658.88	39.22
4N/O	2.08(4)	7(2)				
1S	1.83	21(10)	-13(4)	0.1800	523.64	35.38
3N/O	2.0(1)	8(7)				
2S	2.27(4)	5(3)	-18(8)	0.1462	395.04	82.35
4N/O	2.16(1)	4(1)				
2S	2.68(2)	8(2)	-3(2)	0.1225	256.56	24.09
4N/O	2.12(3)	4(4)				
1S	2.6(1)	3(23)				
1Br	2.5(1)	4(8)	-7(4)	0.0423	111.73	39.94
3N/O	2.11(3)	2(2)				
2S	2.51(8)	13(12)				
1Br	2.44(3)	5(3)	-7(4)	0.0500	135.07	48.29
4N/O	2.10(3)	5(2)				
Im						
1S	2.5(1)	0(14)				
1Br	2.42(8)	2(8)	0(4)	0.0374	108.96	22.71
4N/O	2.10(2)	5(2)				
2Im						
1S	2.46(7)	0(13)				
1Br	2.42(6)	2(8)	0(3)	0.0248	72.16	15.04
4N/O	2.10(3)	5(2)				
3Im						
1S	2.46(9)	0(19)				
1Br	2.43(9)	2(11)	0(3)	0.0304	88.47	18.44
3N/O	2.06(3)	4(2)				
1Im			-5(4)	0.0488	142.18	29.63

2S	2.41(6)	3(5)				
1Br	2.38(5)	2(3)				
3N/O	*2.06(2)*	*4(1)*				
2Im						
2S	*2.41(3)*	*3(3)*				
1Br	*2.38(3)*	*2(2)*	*-5(2)*	*0.0182*	*53.17*	*11.08*
3N/O	**2.05(2)**	**4(2)**				
3Im						
2S	**2.40(4)**	**1(3)**				
1Br	**2.36(4)**	**1(2)**	**-5(3)**	**0.0181**	**52.80**	**11.00**
4N/O	2.10(3)	5(2)				
3Im						
1S	2.46(9)	0(19)				
1Br	2.43(9)	2(11)	0(3)	0.0304	88.47	18.44
4N/O	2.14(2)	4(1)				
1Im						
2S	2.76(7)	13(12)	5(3)	0.1134	330.07	48.55
4N/O	2.14(2)	4(1)				
2Im						
2S	2.8(1)	17(24)	5(2)	0.1169	340.29	50.05

Table S16. Additional Fits for Zn(II) H64C-RcnR in Buffer with 20 mM Hepes, 300 mM NaOAc and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
2N/O	2.14(2)	0(1)	0(4)	0.2859	3005.7	178.93
3N/O	2.14(1)	1(1)	-1(2)	0.1884	2007.66	119.51
4N/O	2.14(1)	3(1)	-2(2)	0.1536	1636.47	97.42
2N/O	2.02(2)	4(2)				
2S	2.265(9)	3.3(7)	-14(2)	0.0374	398.90	26.95
3N/O	2.06(1)	4(1)				
1S	2.285(9)	0.2(7)	-10(2)	0.0367	391.09	26.42
4N/O	2.07(2)	7(1)				
1S	2.28(1)	1.1(9)	-10(2)	0.0451	480.77	32.48
3N/O	2.07(4)	10(3)				
2S	2.26(1)	4(1)	-12(3)	0.0432	460.88	31.14
2N/O	2.00(1)	4(1)				
1Im						
2S	2.272(8)	3.2(4)	-11(2)	0.0104	111.64	16.42
2N/O	2.00(1)	4.0(9)				
2Im						
2S	2.273(7)	3.2(4)	-11(2)	0.0084	89.56	13.17
3N/O	2.03(1)	4.3(7)				
1Im						
1S	2.281(8)	0(0.4)	-8(2)	0.0082	88.33	12.99
3N/O	2.01(1)	4.7(4)				
2Im						
1S	2.275(8)	0.1(4)	-10(2)	0.0082	88.38	13.00
3N/O	2.01(1)	5.0(9)				
3Im						
1S	2.27(1)	0.3(4)	-11(2)	0.0092	98.11	14.43

4N/O	2.04(1)	6.5(7)				
1Im						
1S	2.285(7)	0.5(4)	-6(1)	0.0065	69.45	10.21
4N/O	2.03(9)	6.8(8)				
2Im						
1S	2.281(9)	0.6(4)	-8(2)	0.0072	77.58	11.41
4N/O	2.03(1)	7(1)				
3Im						
1S	2.28(1)	0.7(4)	-9(2)	0.0083	89.24	13.12
3N/O	2.02(2)	7(1)				
1Im						
2S	2.277(8)	3.8(4)	-10(2)	0.0094	100.81	14.83
3N/O	2.02(1)	7(1)				
2Im						
2S	2.279(7)	3.8(4)	-9(2)	0.0075	80.85	11.89
3N/O	**2.02(1)**	**7.0(9)**				
3Im						
2S	**2.280(7)**	**3.8(4)**	**-9(2)**	**0.0067**	**71.9**	**10.57**

Table S17. Additional Fits for Co(II) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
4N/O	2.13(2)	2(1)	-10(4)	0.2306	163.07	9.70
5N/O	2.13(2)	3(1)	-11(3)	0.2097	244.55	14.55
6N/O	2.12(2)	5(1)	-12(3)	0.2054	239.53	14.25
4N/O	2.14(1)	2.1(9)				
1S	2.62(2)	2(2)	-8(3)	0.1286	150.01	10.13
5N/O	2.14(1)	3.5(8)				
1S	2.62(2)	2(2)	-9(2)	0.0974	68.87	4.65
6N/O	2.13(1)	4.8(8)				
1S	2.61(1)	1(1)	-10(2)	0.0822	95.92	6.48
4N/O	2.14(1)	1.9(9)				
2S	2.63(2)	8(3)	-7(2)	0.1344	156.76	10.59
5N/O	2.13(1)	3.2(7)				
1Im						
1S	2.66(2)	0.9(13)	2(2)	0.0382	44.57	6.55
5N/O	2.13(1)	3.2(7)				
2Im						
1S	2.66(2)	0.7(13)	3(2)	0.0377	43.98	6.47
5N/O	2.13(1)	3.2(7)				
3Im						
1S	2.66(1)	0.7(13)	3(2)	0.0380	44.31	6.51
2N/O	2.05(2)	0.5(19)				
3N/O	2.18(2)	0.7(17)				
1Im						
1S	2.63(2)	1(1)	-5(2)	0.0277	32.31	6.73
2N/O	2.05(2)	0.5(18)				
3N/O	2.18(2)	0.7(16)				
2Im			-5(2)	0.0234	27.30	5.69

1S	2.62(1)	1(1)				
3N/O	2.07(2)	2(2)				
2N/O	2.20(2)	0(2)				
1Im						
1S	2.63(1)	1(1)	-3(2)	0.0246	28.74	5.99
3N/O	*2.07(2)*	*2(2)*				
2N/O	*2.20(2)*	*0(2)*				
2Im						
1S	*2.63(1)*	*1(1)*	*-3(2)*	*0.0218*	*25.50*	*5.31*
3N/O	**2.07(2)**	**2(1)**				
2N/O	**2.20(2)**	**0(2)**				
3Im						
1S	**2.63(1)**	**1(1)**	**-4(2)**	**0.0213**	**24.87**	**5.18**
4N/O	2.10(4)	3(3)				
1N/O	2.21(8)	0(7)				
1Im						
1S	2.65(3)	2(3)	-1(7)	0.0700	81.69	17.02
1N/O	2.03(5)	0(4)				
4N/O	2.17(2)	2(2)				
1Im						
1S	2.63(2)	1(2)	-6(3)	0.0463	54.03	11.26

Table S18. Additional Fits for Ni(II) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^{-2})	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
5N/O	2.05(2)	2(1)	-7(3)	0.2229	1862.92	110.90
5N/O	2.07(1)	2(1)				
1S	2.59(4)	4(4)	-4(2)	0.1812	1771.99	119.74
5N/O	2.06(1)	2(1)				
1Im						
1S	2.62(4)	2(4)	7(3)	0.0898	878.38	129.21
5N/O	*2.06(1)*	*2(1)*				
2Im						
1S	*2.62(8)*	*6(8)*	*6(2)*	*0.0715*	*699.46*	*102.89*
5N/O	**2.05(1)**	**2.1(9)**				
3Im						
1S	**2.7(1)**	**5(11)**	**5(2)**	**0.0681**	**666.46**	**98.04**

Table S19. Additional Fits for Ni(II) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaOAc and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r(Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
5N/O	2.08(2)	4(2)	-4(2)	0.2074	910.76	54.21
5N/O	2.087(9)	4.2(8)				
1S	2.62(2)	4(2)	-3(1)	0.0984	487.83	32.96
5N/O	*2.083(7)*	*3.8(5)*				
1Im						
1S	*2.67(2)*	*3(2)*	*9(1)*	*0.0227*	*112.78*	*16.59*
5N/O	**2.083(6)**	**3.8(5)**				
2Im						
1S	**2.67(2)**	**4(2)**	**9(1)**	**0.0223**	**110.93**	**16.31**
5N/O	*2.083(7)*	*3.8(5)*				
3Im						
1S	*2.67(2)*	*4(2)*	*9(1)*	*0.0255*	*111.86*	*16.45*
2N/O	2.07(5)	4(14)				
3N/O	2.09(3)	4(10)				
1Im						
1S	2.63(4)	5(3)	0(2)	0.0221	109.89	22.90
2N/O	2.08(4)	4(13)				
3N/O						
2Im	2.09(2)	4(9)				
1S	2.63(3)	5(3)	2(1)	0.0201	99.68	20.77

Table S20. Additional Fits for Cu(I) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
1N/O	2.12(7)	2(6)	6(9)	0.7731	3213.09	191.28
2N/O	2.13(5)	4(5)	6(5)	0.6820	2834.25	168.72
2N/O	2.09(2)	0.3(19)				
1S	2.37(2)	0(2)	5(2)	0.3049	1217.65	82.28
2N/O	2.4(3)	45(80)				
2S	2.36(2)	5(2)	7(3)	0.4082	1696.46	114.64
1N/O	2.3(2)	0.2(13)				
2S	2.37(5)	4(9)	11(2)	0.4086	1698.31	114.76
2N/O	2.1(1)	20(12)				
1S	2.23(2)	0.9(15)				
1Br	2.47(2)	1.6(6)	-4(5)	0.0717	298.02	23.28
2N/O	2.07(2)	2(2)				
1Im						
2S	2.40(2)	4(1)	13(2)	0.1003	417.20	61.37
2N/O	2.07(2)	2(2)				
2Im						
2S	2.40(2)	4(1)	13(2)	0.1535	638.28	93.89
2N/O	2.09(2)	1(2)				
1Im						
1S	2.41(2)	0(1)	15(3)	0.1021	424.33	62.42
2N/O	2.10(2)	1(2)				
2Im						
1S	2.41(2)	0(1)	16(2)	0.1041	432.70	63.65
1N/O	2.06(4)	0(3)				
1Im						
2S	2.39(3)	4(2)	12(4)	0.1799	747.87	110.01
2N/O	*1.9(1)*	*15(10)*	*-5(5)*	*0.0526*	*218.84*	*45.61*

1Im						
1S	*2.23(3)*	*0.4(1)*				
1Br	*2.47(2)*	*1.3(8)*				
2N/O	1.99(7)	13(9)				
1Im						
1S	2.24(2)	1(2)				
1Br	2.48(2)	1.7(9)	-2(4)	0.0575	239.01	49.81
1N/O	**2.04(3)**	**0(3)**				
1Im						
1S	**2.31(5)**	**3(3)**				
1Br	**2.51(2)**	**3(2)**	**5(5)**	**0.0545**	**217.93**	**45.42**

Table S21. Additional Fits for Zn(II) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaBr and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
4N/O	2.13(2)	4(2)	-9(3)	0.2785	1328.79	79.10
5N/O	2.13(2)	5(1)	-9(3)	0.2383	1136.92	67.68
5N/O	2.15(2)	5(1)				
1S	2.65(4)	8(5)	-7(2)	0.1762	840.58	56.80
4N/O	2.15(2)	4(1)				
2S	2.65(4)	12(6)	-5(2)	0.1904	908.47	61.39
5N/O	2.15(3)	6(3)				
1Br	2.39(8)	13(12)	-8(4)	0.1554	685.43	142.89
4N/O	2.12(3)	4(2)				
1S	2.5(1)	0(17)				
1Br	2.5(1)	3(14)	-8(3)	0.1764	841.53	65.75
5N/O	2.13(1)	5(1)				
1Im						
1S	2.69(4)	6(5)	3(2)	0.0689	328.66	48.34
5N/O	2.13(1)	5(1)				
2Im						
1S	2.67(4)	7(5)	3(2)	0.0556	265.39	39.04
5N/O	2.13(1)	5(1)				
3Im						
1S	2.65(6)	11(9)	2(2)	0.0507	241.88	35.58
3N/O	2.14(2)	4(2)				
2N/O	1.92(4)	22(5)				
1Im						
1S	2.72(4)	6(5)	5(2)	0.0406	193.70	40.37
3N/O	2.14(2)	4(2)				
2N/O	1.92(4)	22(5)				
2Im						
1S	2.72(5)	8(6)	5(2)	0.0341	162.68	33.90

3N/O	2.14(2)	4(2)				
2N/O	1.92(4)	22(5)				
3Im						
1S	2.7(1)	14(14)	5(2)	0.0348	166.40	34.68
4N/O	2.15(2)	6(2)				
1N/O	1.91(4)	14(5)				
1Im						
1S	2.71(4)	6(5)	5(2)	0.0354	169.11	35.24
4N/O	**2.15(2)**	**6(1)**				
1N/O	**1.90(4)**	**14(4)**				
2Im						
1S	**2.69(4)**	**8(5)**	**5(2)**	**0.0263**	**125.75**	**26.20**
4N/O	*2.14(2)*	*5(1)*				
1N/O	*1.90(4)*	*14(5)*				
3Im						
1S	*2.69(6)*	*11(8)*	*4(2)*	*0.0264*	*126.34*	*26.33*
4N/O	2.16(3)	7(3)				
1Im						
1S	1.91(5)	11(5)				
1Br	2.44(4)	12(6)	5(3)	0.0556	265.36	55.31
4N/O	2.17(2)	7(2)				
2Im						
1S	1.91(3)	11(4)				
1Br	2.43(4)	13(5)	6(2)	0.0314	149.8	31.22
5N/O	2.13(2)	6(2)				
1Im						
1Br	2.44(6)	14(8)	2(3)	0.0992	473.19	69.6
5N/O	2.13(2)	5(1)				
2Im						
1Br	2.43(9)	17(12)	1(3)	0.0814	388.36	57.13

Table S22. Additional Fits for Zn(II) H67C-RcnR in Buffer with 20 mM Hepes, 300 mM NaOAc and 10 % Glycerol at pH 7.0.

Data Fit from k = 2-12.5 Å^{-1} and r = 1-4 Å. Numbers in **bold** represent best fits, numbers in *italics* are alternative fits with statistics that are close to the best fits.

N	r (Å)	σ^2 (x10^{-3} Å^2)	ΔE_o (eV)	R factor	χ^2	Reduced χ^2
2N/O	2.11(2)	2(2)	-1(4)	0.3344	5068.61	301.74
3N/O	2.10(2)	4(1)	-2(3)	0.2276	3450.14	205.39
2N/O	2.00(2)	4(1)				
2S	2.26(1)	6(1)	-13(2)	0.0660	1000.86	67.63
3N/O	2.03(2)	4(1)				
1S	2.28(1)	2(1)	-10(2)	0.0683	1035.21	69.95
3N/O	2.02(4)	9(2)				
2S	2.26(2)	8(2)	-12(3)	0.0789	1195.81	80.81
2N/O	**1.981(8)**	**3.6(6)**				
1Im						
2S	**2.271(7)**	**6.0(4)**	**-9(1)**	**0.0061**	**92.77**	**13.64**
2N/O	*1.980(9)*	*3.6(6)*				
2Im						
2S	*2.271(8)*	*6.0(4)*	*-9(1)*	*0.0061*	*93.35*	*13.73*
3N/O	2.02(1)	4.3(7)				
1Im						
1S	2.30(1)	2.3(7)	-4(2)	0.0161	245.27	36.08
3N/O	2.01(1)	4.4(7)				
2Im						
1S	2.30(1)	2.4(7)	-4(2)	0.0132	201.36	29.62
3N/O	2.02(1)	4.4(6)				
3Im						
1S	2.30(1)	2.4(6)	-3(2)	0.0121	1.00	27.05