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Charge Density Distribution and Electrostatic Interactions of Ethionamide: An Inhibitor of enoyl acyl carrier protein reductase (InhA) enzyme of *Mycobacterium tuberculosis*

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Table S1. Geometrical parameters.

Bond lengths (Å)	
C(1) –C(2)	1.3992(3)
C(1)–C(5)	1.4029(3)
C(1)–C(8)	1.4984(3)
C(2)–C(3)	1.3939(4)
C(4)–C(5)	1.4011(3)
C(4)–C(6)	1.5145(4)
C(6)–C(7)	1.5281(5)
N(1)–C(3)	1.3433(4)
N(1)–C(4)	1.3479(4)
N(2)–C(8)	1.3281(4)
S(1)–C(8)	1.6849(3)
C(2)–H(2)	1.0824
C(3)–H(3)	1.0825
C(5)–H(5)	1.0825
C(6)–H(6A)	1.0916
C(6)–H(6B)	1.0926
C(7)–H(7A)	1.0584
C(7)–H(7B)	1.0588
C(7)–H(7C)	1.0592
N(2)–H(2A)	1.0088
N(2)–H(2B)	1.0088
Bond angles (°)	
C(1)–C(2)–C(3)	118.39(2)
C(1)–C(5)–C(4)	119.66(2)
C(2)–C(1)–C(5)	118.29(2)

C(2)–C(1)–C(8)	120.33(2)
C(4)–C(6)–C(7)	116.11(3)
C(5)–C(1)–C(8)	121.34(2)
C(5)–C(4)–C(6)	123.37(2)
C(3)–N(1)–C(4)	118.80(2)
N(1)–C(3)–C(2)	123.37(2)
N(1)–C(3)–H(3)	116.75(2)
N(1)–C(4)–C(5)	121.48(2)
N(1)–C(4)–C(6)	115.14(2)
N(2)–C(8)–C(1)	117.20(2)
S(1)–C(8)–C(1)	120.68(2)
S(1)–C(8)–N(2)	122.10(2)
C(1)–C(2)–H(2)	120.16(2)
C(1)–C(5)–H(5)	120.64(2)
C(2)–C(3)–H(3)	119.87(3)
C(3)–C(2)–H(2)	121.45(2)
C(4)–C(5)–H(5)	119.69(2)
C(4)–C(6)–H(6A)	107.74(3)
C(4)–C(6)–H(6B)	109.37(3)
C(6)–C(7)–H(7A)	114.21(3)
C(6)–C(7)–H(7B)	110.73(3)
C(6)–C(7)–H(7C)	106.02(3)
C(7)–C(6)–H(6A)	112.50(3)
C(7)–C(6)–H(6B)	109.17(3)
C(8)–N(2)–H(2A)	119.29(3)
C(8)–N(2)–H(2B)	122.19(3)
H(2A)–N(2)–H(2B)	118.44(3)
H(6A)–C(6)–H(6B)	100.83(3)
H(7A)–C(7)–H(7B)	108.17(3)
H(7A)–C(7)–H(7C)	108.92(3)
H(7B)–C(7)–H(7C)	108.65(3)

Torsion angles (°)

C(4)–N(1)–C(3)–C(2)	0.7(1)
C(3)–N(1)–C(4)–C(5)	-1.2(1)
C(3)–N(1)–C(4)–C(6)	177.4(1)
C(4)–N(1)–C(3)–H(3)	-178.0(1)
H(2A)–N(2)–C(8)–S(1)	4.3(1)
H(2A)–N(2)–C(8)–C(1)	-173.8(1)
H(2B)–N(2)–C(8)–S(1)	-172.4(1)
H(2B)–N(2)–C(8)–C(1)	9.5(1)
C(5)–C(1)–C(2)–C(3)	-0.6(1)
C(2)–C(1)–C(5)–C(4)	0.2(1)
C(5)–C(1)–C(2)–H(2)	179.2(1)
C(2)–C(1)–C(5)–H(5)	-179.0(1)
C(2)–C(1)–C(8)–S(1)	27.0(1)

C(2)–C(1)–C(8)–N(2)	-154.9(1)
C(8)–C(1)–C(2)–C(3)	-178.2(1)
C(8)–C(1)–C(2)–H(2)	1.6(1)
C(5)–C(1)–C(8)–S(1)	-150.5(1)
C(5)–C(1)–C(8)–N(2)	27.6(1)
C(8)–C(1)–C(5)–C(4)	177.8(1)
C(8)–C(1)–C(5)–H(5)	-1.4(1)
C(1)–C(2)–C(3)–N(1)	0.2(1)
C(1)–C(2)–C(3)–H(3)	178.8(1)
H(2)–C(2)–C(3)–N(1)	-179.6(1)
H(2)–C(2)–C(3)–H(3)	-1.0(1)
N(1)–C(4)–C(5)–C(1)	0.7(1)
N(1)–C(4)–C(5)–H(5)	179.9(1)
N(1)–C(4)–C(6)–C(7)	176.9(1)
N(1)–C(4)–C(6)–H(6A)	-55.9(1)
N(1)–C(4)–C(6)–H(6B)	52.9(1)
C(6)–C(4)–C(5)–C(1)	-177.8(1)
C(5)–C(4)–C(6)–C(7)	-4.5(1)
C(6)–C(4)–C(5)–H(5)	1.5(1)
C(5)–C(4)–C(6)–H(6A)	122.7(1)
C(5)–C(4)–C(6)–H(6B)	-128.6(1)
C(4)–C(6)–C(7)–H(7A)	60.7(1)
C(4)–C(6)–C(7)–H(7B)	-61.7(1)
C(4)–C(6)–C(7)–H(7C)	-179.4(1)
H(6A)–C(6)–C(7)–H(7A)	-64.1(1)
H(6A)–C(6)–C(7)–H(7B)	173.5(1)
H(6A)–C(6)–C(7)–H(7C)	55.8(1)
H(6B)–C(6)–C(7)–H(7A)	-175.2(1)
H(6B)–C(6)–C(7)–H(7B)	62.4(1)
H(6B)–C(6)–C(7)–H(7C)	-55.2(1)

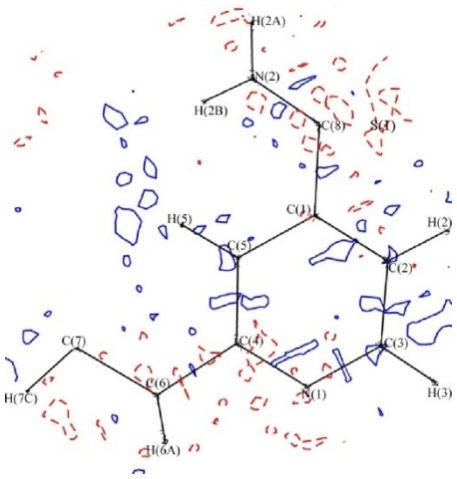

Fig S1: Residual map of ethionamide, in the plane of C(7), C(4), N(2) atoms and solid lines show the positive contours and dashed lines are negative contours. The contours are drawn at ± 0.05 eÅ^{-3} intervals.