Table 1. Crystal data and structure refinement for p1.

Identification code	p1
Empirical formula	C31 H35 Fe N O5
Formula weight	557.45
Temperature	291(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 7.4950(15) A alpha = 97.02(3) deg. b = 8.1766(16) A beta = 98.63(3) deg. c = 12.237(2) A gamma = 109.63(3) deg.
Volume	686.3(2) A^3
Z, Calculated density	1, 1.349 Mg/m^3
Absorption coefficient	0.590 mm^-1
F(000)	294
Crystal size	0.20 x 0.18 x 0.17 mm
Theta range for data collection	1.71 to 25.50 deg.
Limiting indices	-8<=h<=7, 0<=k<=9, -14<=l<=14
Reflections collected / unique	2381 / 2381 [R(int) = 0.0000]
Completeness to theta = 25.50	93.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9063 and 0.8911
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2381 / 3 / 352
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0797

R indices (all data)	R1 = 0.0381, wR2 = 0.0824
Absolute structure parameter	0.088(19)
Extinction coefficient	0.092(6)
Largest diff. peak and hole	0.263 and -0.327 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for p1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	17148(1)	7728(1)	5404(1)	40(1)
O(1)	15930(5)	11193(4)	10938(3)	43(1)
O(2)	12359(5)	9388(4)	9595(3)	57(1)
O(3)	13260(4)	7551(4)	8520(3)	49(1)
O(4)	5491(5)	4580(5)	7906(4)	67(1)
O(5)	2391(6)	4169(6)	7707(5)	74(1)
N(1)	16952(5)	9937(4)	8872(3)	33(1)
C(1)	17489(11)	5413(9)	5456(6)	67(2)
C(2)	16810(8)	5476(8)	4366(5)	57(1)
C(3)	18108(8)	6900(8)	4050(5)	54(1)
C(4)	19659(8)	7739(9)	4947(5)	59(2)
C(5)	19307(10)	6817(9)	5845(5)	63(2)
C(6)	14892(6)	7806(7)	6150(4)	45(1)
C(7)	14654(7)	8280(8)	5086(5)	54(1)
C(8)	16250(9)	9795(9)	5066(4)	58(2)
C(9)	17534(8)	10271(7)	6144(5)	48(1)
C(10)	16710(7)	9029(6)	6822(4)	37(1)
C(11)	17590(6)	8941(5)	7979(3)	36(1)
C(12)	17605(7)	11900(5)	8878(4)	46(1)
C(13)	19194(7)	12243(6)	9907(4)	46(1)
C(14)	18219(6)	10310(5)	10045(3)	33(1)
C(15)	17140(5)	10172(5)	11030(3)	33(1)
C(16)	15951(6)	8272(5)	11134(3)	36(1)
C(17)	16272(8)	6809(6)	10664(4)	55(1)
C(18)	15257(11)	5137(7)	10863(5)	70(2)
C(19)	13900(9)	4915(7)	11504(5)	68(2)
C(20)	13532(8)	6347(8)	11956(4)	64(2)
C(21)	14538(7)	8039(7)	11782(4)	51(1)
C(22)	18714(6)	11046(5)	12103(3)	37(1)
C(23)	20212(6)	10432(6)	12367(4)	47(1)
C(24)	21664(9)	11213(9)	13323(5)	59(2)
C(25)	21578(8)	12616(7)	14050(4)	62(1)
C(26)	20122(9)	13242(8)	13814(5)	64(1)
C(27)	18693(7)	12469(6)	12834(4)	51(1)
C(28)	12117(6)	7875(6)	9102(3)	40(1)
C(29)	10407(7)	6344(7)	9194(5)	60(1)
C(30)	3819(7)	3622(6)	7626(4)	48(1)

C(31)	3179(8)	1700(8)	7183(6)	68(2)

Table 3. Bond lengths [A] and angles [deg] for p1.

Fe(1)-C(1)	2.000(6)
Fe(1)-C(2)	2.021(6)
Fe(1)-C(5)	2.027(6)
Fe(1)-C(3)	2.032(5)
Fe(1)-C(4)	2.040(6)
Fe(1)-C(10)	2.051(5)
Fe(1)-C(6)	2.054(5)
Fe(1)-C(7)	2.059(5)
Fe(1)-C(9)	2.070(6)
Fe(1)-C(8)	2.081(6)
O(1)-C(15)	1.426(5)
O(1)-H(1E)	0.87(6)
O(2)-C(28)	1.249(5)
O(3)-C(28)	1.265(5)
O(4)-C(30)	1.203(6)
O(5)-C(30)	1.304(6)
O(5)-H(5B)	0.8200
N(1)-C(12)	1.511(5)
N(1)-C(11)	1.513(5)
N(1)-C(14)	1.531(5)
N(1)-H(1F)	0.89(5)
C(1)-C(2)	1.368(9)
C(1)-C(5)	1.422(10)
C(1)-H(1A)	0.9800
C(2)-C(3)	1.383(8)
C(2)-H(2A)	0.9800
C(3)-C(4)	1.387(8)
C(3)-H(3A)	0.9800
C(4)-C(5)	1.415(10)
C(4)-H(4A)	0.9800
C(5)-H(5A)	0.9800
C(6)-C(7)	1.406(8)
C(6)-C(10)	1.443(7)
C(6)-H(6A)	0.9800
C(7)-C(8)	1.409(9)
C(7)-H(7A)	0.9800
C(8)-C(9)	1.435(8)
C(8)-H(8A)	0.9800
C(9)-C(10)	1.429(7)
C(9)-H(9A)	0.9800
C(10)-C(11)	1.490(6)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.524(6)

C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.545(6)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.544(5)
C(14)-H(14A)	0.9800
C(15)-C(22)	1.538(6)
C(15)-C(16)	1.541(5)
C(16)-C(17)	1.374(6)
C(16)-C(21)	1.393(6)
C(17)-C(18)	1.395(8)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.354(9)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.363(9)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.396(7)
C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9300
C(22)-C(27)	1.385(6)
C(22)-C(23)	1.388(6)
C(23)-C(24)	1.389(7)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.389(9)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.362(9)
C(25)-H(25A)	0.9300
C(26)-C(27)	1.400(8)
C(26)-H(26A)	0.9300
C(27)-H(27A)	0.9300
C(28)-C(29)	1.491(6)
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-C(31)	1.483(7)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600

C(1)-Fe(1)-C(2)	39.8(3)
C(1)-Fe(1)-C(5)	41.3(3)
C(2)-Fe(1)-C(5)	67.8(3)
C(1)-Fe(1)-C(3)	67.6(3)
C(2)-Fe(1)-C(3)	39.9(2)
C(5)-Fe(1)-C(3)	67.7(2)
C(1)-Fe(1)-C(4)	68.5(3)
C(2)-Fe(1)-C(4)	67.2(2)

C(5)-Fe(1)-C(4)	40.7(3)
C(3)-Fe(1)-C(4)	39.8(2)
C(1)-Fe(1)-C(10)	118.5(2)
C(2)-Fe(1)-C(10)	151.2(2)
C(5)-Fe(1)-C(10)	109.0(2)
C(3)-Fe(1)-C(10)	167.7(2)
C(4)-Fe(1)-C(10)	130.1(2)
C(1)-Fe(1)-C(6)	109.7(2)
C(2)-Fe(1)-C(6)	118.2(2)
C(5)-Fe(1)-C(6)	131.4(2)
C(3)-Fe(1)-C(6)	149.7(2)
C(4)-Fe(1)-C(6)	169.9(2)
C(10)-Fe(1)-C(6)	41.16(19)
C(1)-Fe(1)-C(7)	129.9(3)
C(2)-Fe(1)-C(7)	109.2(2)
C(5)-Fe(1)-C(7)	169.4(3)
C(3)-Fe(1)-C(7)	117.1(2)
C(4)-Fe(1)-C(7)	148.8(3)
C(10)-Fe(1)-C(7)	68.3(2)
C(6)-Fe(1)-C(7)	40.0(2)
C(1)-Fe(1)-C(9)	151.6(3)
C(2)-Fe(1)-C(9)	167.2(2)
C(5)-Fe(1)-C(9)	117.7(3)
C(3)-Fe(1)-C(9)	129.3(2)
C(4)-Fe(1)-C(9)	108.6(2)
C(10)-Fe(1)-C(9)	40.56(19)
C(6)-Fe(1)-C(9)	67.9(2)
C(7)-Fe(1)-C(9)	67.5(2)
C(1)-Fe(1)-C(8)	167.0(3)
C(2)-Fe(1)-C(8)	129.3(2)
C(5)-Fe(1)-C(8)	149.9(3)
C(3)-Fe(1)-C(8)	108.2(2)
C(4)-Fe(1)-C(8)	116.7(3)
C(10)-Fe(1)-C(8)	68.3(2)
C(6)-Fe(1)-C(8)	67.4(2)
C(7)-Fe(1)-C(8)	39.8(3)
C(9)-Fe(1)-C(8)	40.4(2)
C(15)-O(1)-H(1E)	109(4)
C(30)-O(5)-H(5B)	109.5
C(12)-N(1)-C(11)	113.4(3)
C(12)-N(1)-C(14)	89.7(3)
C(11)-N(1)-C(14)	113.3(3)
C(12)-N(1)-H(1F)	114(3)
C(11)-N(1)-H(1F)	105(3)
C(14)-N(1)-H(1F)	122(3)
C(2)-C(1)-C(5)	108.0(5)
C(2)-C(1)-Fe(1)	70.9(4)
C(5)-C(1)-Fe(1)	70.3(4)

C(2)-C(1)-H(1A)	126.0
C(5)-C(1)-H(1A)	126.0
Fe(1)-C(1)-H(1A)	126.0
C(1)-C(2)-C(3)	109.1(6)
C(1)-C(2)-Fe(1)	69.3(4)
C(3)-C(2)-Fe(1)	70.5(3)
C(1)-C(2)-H(2A)	125.4
C(3)-C(2)-H(2A)	125.4
Fe(1)-C(2)-H(2A)	125.4
C(2)-C(3)-C(4)	108.6(6)
C(2)-C(3)-Fe(1)	69.6(3)
C(4)-C(3)-Fe(1)	70.4(3)
C(2)-C(3)-H(3A)	125.7
C(4)-C(3)-H(3A)	125.7
Fe(1)-C(3)-H(3A)	125.7
C(3)-C(4)-C(5)	107.7(6)
C(3)-C(4)-Fe(1)	69.8(3)
C(5)-C(4)-Fe(1)	69.2(3)
C(3)-C(4)-H(4A)	126.1
C(5)-C(4)-H(4A)	126.1
Fe(1)-C(4)-H(4A)	126.1
C(4)-C(5)-C(1)	106.5(5)
C(4)-C(5)-Fe(1)	70.1(3)
C(1)-C(5)-Fe(1)	68.3(3)
C(4)-C(5)-H(5A)	126.7
C(1)-C(5)-H(5A)	126.7
Fe(1)-C(5)-H(5A)	126.7
C(7)-C(6)-C(10)	108.3(4)
C(7)-C(6)-Fe(1)	70.2(3)
C(10)-C(6)-Fe(1)	69.3(2)
C(7)-C(6)-H(6A)	125.9
C(10)-C(6)-H(6A)	125.9
Fe(1)-C(6)-H(6A)	125.9
C(6)-C(7)-C(8)	109.1(5)
C(6)-C(7)-Fe(1)	69.8(3)
C(8)-C(7)-Fe(1)	70.9(3)
C(6)-C(7)-H(7A)	125.4
C(8)-C(7)-H(7A)	125.4
Fe(1)-C(7)-H(7A)	125.4
C(7)-C(8)-C(9)	107.6(5)
C(7)-C(8)-Fe(1)	69.3(3)
C(9)-C(8)-Fe(1)	69.4(3)
C(7)-C(8)-H(8A)	126.2
C(9)-C(8)-H(8A)	126.2
Fe(1)-C(8)-H(8A)	126.2
C(10)-C(9)-C(8)	108.2(5)
C(10)-C(9)-Fe(1)	69.0(3)
C(8)-C(9)-Fe(1)	70.2(3)

C(10)-C(9)-H(9A)	125.9
C(8)-C(9)-H(9A)	125.9
Fe(1)-C(9)-H(9A)	125.9
C(9)-C(10)-C(6)	106.8(5)
C(9)-C(10)-C(11)	127.1(5)
C(6)-C(10)-C(11)	126.1(4)
C(9)-C(10)-Fe(1)	70.4(3)
C(6)-C(10)-Fe(1)	69.5(3)
C(11)-C(10)-Fe(1)	122.7(3)
C(10)-C(11)-N(1)	112.0(3)
C(10)-C(11)-H(11A)	109.2
N(1)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11B)	109.2
N(1)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
N(1)-C(12)-C(13)	90.3(3)
N(1)-C(12)-H(12A)	113.6
C(13)-C(12)-H(12A)	113.6
N(1)-C(12)-H(12B)	113.6
C(13)-C(12)-H(12B)	113.6
H(12A)-C(12)-H(12B)	110.9
C(12)-C(13)-C(14)	88.7(3)
C(12)-C(13)-H(13A)	113.9
C(14)-C(13)-H(13A)	113.9
C(12)-C(13)-H(13B)	113.9
C(14)-C(13)-H(13B)	113.9
H(13A)-C(13)-H(13B)	111.1
N(1)-C(14)-C(15)	115.7(3)
N(1)-C(14)-C(13)	88.8(3)
C(15)-C(14)-C(13)	112.3(3)
N(1)-C(14)-H(14A)	112.7
C(15)-C(14)-H(14A)	112.7
C(13)-C(14)-H(14A)	112.7
O(1)-C(15)-C(22)	107.5(3)
O(1)-C(15)-C(16)	110.2(3)
C(22)-C(15)-C(16)	109.1(3)
O(1)-C(15)-C(14)	109.1(3)
C(22)-C(15)-C(14)	105.8(3)
C(16)-C(15)-C(14)	114.9(3)
C(17)-C(16)-C(21)	118.4(4)
C(17)-C(16)-C(15)	123.4(4)
C(21)-C(16)-C(15)	118.1(4)
C(16)-C(17)-C(18)	120.8(5)
C(16)-C(17)-H(17A)	119.6
C(18)-C(17)-H(17A)	119.6
C(19)-C(18)-C(17)	120.7(6)
C(19)-C(18)-H(18A)	119.7
C(17)-C(18)-H(18A)	119.7

C(18)-C(19)-C(20)	119.3(5)
C(18)-C(19)-H(19A)	120.4
C(20)-C(19)-H(19A)	120.4
C(19)-C(20)-C(21)	121.4(5)
C(19)-C(20)-H(20A)	119.3
C(21)-C(20)-H(20A)	119.3
C(16)-C(21)-C(20)	119.4(5)
C(16)-C(21)-H(21A)	120.3
C(20)-C(21)-H(21A)	120.3
C(27)-C(22)-C(23)	117.8(4)
C(27)-C(22)-C(15)	121.4(4)
C(23)-C(22)-C(15)	120.8(4)
C(22)-C(23)-C(24)	121.9(5)
C(22)-C(23)-H(23A)	119.0
C(24)-C(23)-H(23A)	119.0
C(23)-C(24)-C(25)	118.8(6)
C(23)-C(24)-H(24A)	120.6
C(25)-C(24)-H(24A)	120.6
C(26)-C(25)-C(24)	120.5(5)
C(26)-C(25)-H(25A)	119.7
C(24)-C(25)-H(25A)	119.7
C(25)-C(26)-C(27)	120.0(5)
C(25)-C(26)-H(26A)	120.0
C(27)-C(26)-H(26A)	120.0
C(22)-C(27)-C(26)	120.9(5)
C(22)-C(27)-H(27A)	119.6
C(26)-C(27)-H(27A)	119.6
O(2)-C(28)-O(3)	123.5(4)
O(2)-C(28)-C(29)	119.5(4)
O(3)-C(28)-C(29)	117.0(4)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(4)-C(30)-O(5)	123.0(5)
O(4)-C(30)-C(31)	123.5(4)
O(5)-C(30)-C(31)	113.4(4)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for p1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	37(1)	55(1)	31(1)	7(1)	10(1)	20(1)
O(1)	40(2)	32(2)	58(2)	2(1)	7(1)	17(1)
O(2)	49(2)	44(2)	75(2)	0(2)	3(2)	21(1)
O(3)	36(2)	44(2)	63(2)	6(1)	17(1)	8(1)
O(4)	43(2)	48(2)	101(3)	12(2)	9(2)	6(2)
O(5)	57(3)	53(2)	106(4)	-3(2)	13(2)	20(2)
N(1)	32(2)	28(2)	35(2)	5(1)	5(1)	9(1)
C(1)	87(5)	71(4)	71(4)	29(3)	47(4)	44(3)
C(2)	47(3)	56(3)	61(4)	0(3)	11(2)	13(2)
C(3)	55(3)	72(4)	38(3)	3(2)	15(2)	28(3)
C(4)	45(3)	67(3)	58(4)	-8(3)	14(2)	18(2)
C(5)	73(4)	94(5)	39(3)	-3(3)	3(3)	59(4)
C(6)	21(2)	67(3)	46(3)	8(2)	11(2)	15(2)
C(7)	30(2)	80(4)	48(3)	6(3)	1(2)	21(2)
C(8)	75(4)	80(4)	38(3)	23(3)	16(3)	49(3)
C(9)	55(3)	48(3)	49(3)	16(2)	24(2)	24(2)
C(10)	37(2)	46(3)	33(2)	6(2)	11(2)	19(2)
C(11)	38(2)	40(2)	34(2)	7(2)	12(2)	18(2)
C(12)	63(3)	29(2)	42(2)	9(2)	3(2)	14(2)
C(13)	52(2)	38(2)	37(2)	10(2)	5(2)	2(2)
C(14)	37(2)	32(2)	30(2)	9(2)	5(2)	11(2)
C(15)	36(2)	26(2)	37(2)	5(2)	7(1)	11(2)
C(16)	41(2)	31(2)	29(2)	4(2)	5(1)	9(2)
C(17)	78(3)	38(2)	60(3)	13(2)	31(2)	27(2)
C(18)	105(5)	33(3)	65(4)	9(2)	12(3)	17(3)
C(19)	76(4)	47(3)	53(3)	24(2)	-11(3)	-7(2)
C(20)	51(3)	75(4)	49(3)	24(3)	9(2)	-2(2)
C(21)	48(3)	56(3)	41(2)	10(2)	13(2)	9(2)
C(22)	41(2)	31(2)	34(2)	4(2)	11(2)	5(2)
C(23)	45(2)	43(2)	49(2)	5(2)	3(2)	15(2)
C(24)	53(3)	69(4)	46(3)	13(3)	-4(2)	16(3)
C(25)	61(3)	63(3)	42(3)	2(2)	1(2)	3(2)
C(26)	71(4)	63(3)	48(3)	-9(2)	12(2)	19(3)
C(27)	47(3)	46(3)	53(3)	-2(2)	10(2)	15(2)
C(28)	35(2)	45(2)	44(2)	12(2)	6(2)	20(2)
C(29)	35(2)	56(3)	95(4)	25(3)	26(2)	16(2)
C(30)	52(3)	50(3)	45(2)	13(2)	9(2)	20(2)
C(31)	54(3)	55(3)	83(4)	-8(3)	-3(3)	20(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for p1.

	x	y	z	U(eq)
H(5B)	2822	5232	7965	111
H(1A)	16855	4530	5886	81
H(2A)	15587	4658	3890	69
H(3A)	17955	7258	3317	65
H(4A)	20792	8788	4958	70
H(5A)	20154	7088	6587	76
H(6A)	13983	6811	6391	54
H(7A)	13554	7658	4459	65
H(8A)	16454	10404	4428	69
H(9A)	18770	11268	6372	57
H(11A)	18989	9436	8084	43
H(11B)	17225	7714	8064	43
H(12A)	16642	12406	9016	55
H(12B)	18092	12233	8215	55
H(13A)	19198	13111	10524	56
H(13B)	20475	12507	9739	56
H(14A)	19112	9666	10081	40
H(17A)	17178	6935	10207	66
H(18A)	15514	4165	10552	84
H(19A)	13227	3798	11635	81
H(20A)	12590	6193	12389	77
H(21A)	14268	9002	12095	61
H(23A)	20243	9469	11891	56
H(24A)	22677	10805	13473	71
H(25A)	22522	13131	14704	74
H(26A)	20077	14184	14305	76
H(27A)	17716	12918	12671	61
H(29A)	9654	6749	9655	90
H(29B)	10837	5504	9528	90
H(29C)	9627	5793	8458	90
H(31A)	4290	1380	7137	101
H(31B)	2373	1425	6448	101
H(31C)	2460	1051	7677	101
H(1E)	14790(90)	10520(70)	10550(50)	54(15)
H(1F)	15670(80)	9400(60)	8740(40)	40(12)

Table 6. Torsion angles [deg] for p1.

C(5)-Fe(1)-C(1)-C(2)	-118.1(5)
C(3)-Fe(1)-C(1)-C(2)	-36.8(4)
C(4)-Fe(1)-C(1)-C(2)	-79.9(4)
C(10)-Fe(1)-C(1)-C(2)	155.1(3)
C(6)-Fe(1)-C(1)-C(2)	110.8(4)
C(7)-Fe(1)-C(1)-C(2)	70.5(5)
C(9)-Fe(1)-C(1)-C(2)	-169.4(5)
C(8)-Fe(1)-C(1)-C(2)	36.4(14)
C(2)-Fe(1)-C(1)-C(5)	118.1(5)
C(3)-Fe(1)-C(1)-C(5)	81.3(4)
C(4)-Fe(1)-C(1)-C(5)	38.2(3)
C(10)-Fe(1)-C(1)-C(5)	-86.8(4)
C(6)-Fe(1)-C(1)-C(5)	-131.1(3)
C(7)-Fe(1)-C(1)-C(5)	-171.4(4)
C(9)-Fe(1)-C(1)-C(5)	-51.3(6)
C(8)-Fe(1)-C(1)-C(5)	154.5(11)
C(5)-C(1)-C(2)-C(3)	-1.5(7)
Fe(1)-C(1)-C(2)-C(3)	59.4(4)
C(5)-C(1)-C(2)-Fe(1)	-60.9(4)
C(5)-Fe(1)-C(2)-C(1)	39.0(4)
C(3)-Fe(1)-C(2)-C(1)	120.4(5)
C(4)-Fe(1)-C(2)-C(1)	83.2(4)
C(10)-Fe(1)-C(2)-C(1)	-50.2(6)
C(6)-Fe(1)-C(2)-C(1)	-87.3(4)
C(7)-Fe(1)-C(2)-C(1)	-130.1(4)
C(9)-Fe(1)-C(2)-C(1)	156.8(11)
C(8)-Fe(1)-C(2)-C(1)	-170.1(4)
C(1)-Fe(1)-C(2)-C(3)	-120.4(5)
C(5)-Fe(1)-C(2)-C(3)	-81.4(4)
C(4)-Fe(1)-C(2)-C(3)	-37.2(4)
C(10)-Fe(1)-C(2)-C(3)	-170.7(4)
C(6)-Fe(1)-C(2)-C(3)	152.3(3)
C(7)-Fe(1)-C(2)-C(3)	109.5(4)
C(9)-Fe(1)-C(2)-C(3)	36.4(14)
C(8)-Fe(1)-C(2)-C(3)	69.5(4)
C(1)-C(2)-C(3)-C(4)	1.2(7)
Fe(1)-C(2)-C(3)-C(4)	59.9(4)
C(1)-C(2)-C(3)-Fe(1)	-58.6(4)
C(1)-Fe(1)-C(3)-C(2)	36.7(4)
C(5)-Fe(1)-C(3)-C(2)	81.5(4)
C(4)-Fe(1)-C(3)-C(2)	119.5(6)
C(10)-Fe(1)-C(3)-C(2)	158.4(11)
C(6)-Fe(1)-C(3)-C(2)	-54.2(6)
C(7)-Fe(1)-C(3)-C(2)	-88.0(4)

C(9)-Fe(1)-C(3)-C(2)	-170.2(4)
C(8)-Fe(1)-C(3)-C(2)	-130.3(4)
C(1)-Fe(1)-C(3)-C(4)	-82.9(5)
C(2)-Fe(1)-C(3)-C(4)	-119.5(5)
C(5)-Fe(1)-C(3)-C(4)	-38.0(4)
C(10)-Fe(1)-C(3)-C(4)	38.9(14)
C(6)-Fe(1)-C(3)-C(4)	-173.7(5)
C(7)-Fe(1)-C(3)-C(4)	152.5(4)
C(9)-Fe(1)-C(3)-C(4)	70.3(5)
C(8)-Fe(1)-C(3)-C(4)	110.2(4)
C(2)-C(3)-C(4)-C(5)	-0.4(7)
Fe(1)-C(3)-C(4)-C(5)	59.0(4)
C(2)-C(3)-C(4)-Fe(1)	-59.4(4)
C(1)-Fe(1)-C(4)-C(3)	80.3(4)
C(2)-Fe(1)-C(4)-C(3)	37.3(4)
C(5)-Fe(1)-C(4)-C(3)	119.1(5)
C(10)-Fe(1)-C(4)-C(3)	-170.0(4)
C(6)-Fe(1)-C(4)-C(3)	161.7(15)
C(7)-Fe(1)-C(4)-C(3)	-52.6(6)
C(9)-Fe(1)-C(4)-C(3)	-129.8(4)
C(8)-Fe(1)-C(4)-C(3)	-86.6(4)
C(1)-Fe(1)-C(4)-C(5)	-38.8(4)
C(2)-Fe(1)-C(4)-C(5)	-81.9(4)
C(3)-Fe(1)-C(4)-C(5)	-119.1(5)
C(10)-Fe(1)-C(4)-C(5)	70.9(5)
C(6)-Fe(1)-C(4)-C(5)	42.5(18)
C(7)-Fe(1)-C(4)-C(5)	-171.7(5)
C(9)-Fe(1)-C(4)-C(5)	111.0(4)
C(8)-Fe(1)-C(4)-C(5)	154.2(4)
C(3)-C(4)-C(5)-C(1)	-0.5(7)
Fe(1)-C(4)-C(5)-C(1)	58.9(4)
C(3)-C(4)-C(5)-Fe(1)	-59.4(4)
C(2)-C(1)-C(5)-C(4)	1.2(7)
Fe(1)-C(1)-C(5)-C(4)	-60.0(4)
C(2)-C(1)-C(5)-Fe(1)	61.2(4)
C(1)-Fe(1)-C(5)-C(4)	118.0(5)
C(2)-Fe(1)-C(5)-C(4)	80.4(4)
C(3)-Fe(1)-C(5)-C(4)	37.2(3)
C(10)-Fe(1)-C(5)-C(4)	-130.2(3)
C(6)-Fe(1)-C(5)-C(4)	-170.9(4)
C(7)-Fe(1)-C(5)-C(4)	156.2(14)
C(9)-Fe(1)-C(5)-C(4)	-86.8(4)
C(8)-Fe(1)-C(5)-C(4)	-50.9(6)
C(2)-Fe(1)-C(5)-C(1)	-37.6(4)
C(3)-Fe(1)-C(5)-C(1)	-80.8(4)
C(4)-Fe(1)-C(5)-C(1)	-118.0(5)
C(10)-Fe(1)-C(5)-C(1)	111.8(4)
C(6)-Fe(1)-C(5)-C(1)	71.1(4)

C(7)-Fe(1)-C(5)-C(1)	38.2(16)
C(9)-Fe(1)-C(5)-C(1)	155.2(3)
C(8)-Fe(1)-C(5)-C(1)	-168.9(5)
C(1)-Fe(1)-C(6)-C(7)	-129.4(4)
C(2)-Fe(1)-C(6)-C(7)	-86.7(4)
C(5)-Fe(1)-C(6)-C(7)	-171.0(4)
C(3)-Fe(1)-C(6)-C(7)	-50.5(6)
C(4)-Fe(1)-C(6)-C(7)	153.0(16)
C(10)-Fe(1)-C(6)-C(7)	119.5(5)
C(9)-Fe(1)-C(6)-C(7)	80.9(4)
C(8)-Fe(1)-C(6)-C(7)	37.0(4)
C(1)-Fe(1)-C(6)-C(10)	111.1(4)
C(2)-Fe(1)-C(6)-C(10)	153.8(3)
C(5)-Fe(1)-C(6)-C(10)	69.5(4)
C(3)-Fe(1)-C(6)-C(10)	-170.0(5)
C(4)-Fe(1)-C(6)-C(10)	33.5(18)
C(7)-Fe(1)-C(6)-C(10)	-119.5(5)
C(9)-Fe(1)-C(6)-C(10)	-38.6(3)
C(8)-Fe(1)-C(6)-C(10)	-82.4(3)
C(10)-C(6)-C(7)-C(8)	-1.2(6)
Fe(1)-C(6)-C(7)-C(8)	-60.3(4)
C(10)-C(6)-C(7)-Fe(1)	59.1(3)
C(1)-Fe(1)-C(7)-C(6)	71.6(4)
C(2)-Fe(1)-C(7)-C(6)	111.3(4)
C(5)-Fe(1)-C(7)-C(6)	39.4(17)
C(3)-Fe(1)-C(7)-C(6)	154.0(3)
C(4)-Fe(1)-C(7)-C(6)	-171.1(5)
C(10)-Fe(1)-C(7)-C(6)	-38.1(3)
C(9)-Fe(1)-C(7)-C(6)	-82.0(3)
C(8)-Fe(1)-C(7)-C(6)	-119.7(5)
C(1)-Fe(1)-C(7)-C(8)	-168.7(4)
C(2)-Fe(1)-C(7)-C(8)	-129.0(3)
C(5)-Fe(1)-C(7)-C(8)	159.1(14)
C(3)-Fe(1)-C(7)-C(8)	-86.2(4)
C(4)-Fe(1)-C(7)-C(8)	-51.4(6)
C(10)-Fe(1)-C(7)-C(8)	81.7(3)
C(6)-Fe(1)-C(7)-C(8)	119.7(5)
C(9)-Fe(1)-C(7)-C(8)	37.8(3)
C(6)-C(7)-C(8)-C(9)	0.6(7)
Fe(1)-C(7)-C(8)-C(9)	-59.0(4)
C(6)-C(7)-C(8)-Fe(1)	59.6(4)
C(1)-Fe(1)-C(8)-C(7)	42.1(13)
C(2)-Fe(1)-C(8)-C(7)	71.5(4)
C(5)-Fe(1)-C(8)-C(7)	-172.4(5)
C(3)-Fe(1)-C(8)-C(7)	110.7(4)
C(4)-Fe(1)-C(8)-C(7)	153.0(3)
C(10)-Fe(1)-C(8)-C(7)	-81.8(4)
C(6)-Fe(1)-C(8)-C(7)	-37.2(3)

C(9)-Fe(1)-C(8)-C(7)	-119.2(5)
C(1)-Fe(1)-C(8)-C(9)	161.3(10)
C(2)-Fe(1)-C(8)-C(9)	-169.3(3)
C(5)-Fe(1)-C(8)-C(9)	-53.2(6)
C(3)-Fe(1)-C(8)-C(9)	-130.0(3)
C(4)-Fe(1)-C(8)-C(9)	-87.7(4)
C(10)-Fe(1)-C(8)-C(9)	37.5(3)
C(6)-Fe(1)-C(8)-C(9)	82.1(3)
C(7)-Fe(1)-C(8)-C(9)	119.2(5)
C(7)-C(8)-C(9)-C(10)	0.2(6)
Fe(1)-C(8)-C(9)-C(10)	-58.7(4)
C(7)-C(8)-C(9)-Fe(1)	58.9(4)
C(1)-Fe(1)-C(9)-C(10)	-51.7(6)
C(2)-Fe(1)-C(9)-C(10)	160.3(11)
C(5)-Fe(1)-C(9)-C(10)	-87.3(4)
C(3)-Fe(1)-C(9)-C(10)	-170.2(3)
C(4)-Fe(1)-C(9)-C(10)	-130.7(3)
C(6)-Fe(1)-C(9)-C(10)	39.1(3)
C(7)-Fe(1)-C(9)-C(10)	82.5(3)
C(8)-Fe(1)-C(9)-C(10)	119.6(5)
C(1)-Fe(1)-C(9)-C(8)	-171.3(5)
C(2)-Fe(1)-C(9)-C(8)	40.7(14)
C(5)-Fe(1)-C(9)-C(8)	153.1(4)
C(3)-Fe(1)-C(9)-C(8)	70.2(4)
C(4)-Fe(1)-C(9)-C(8)	109.7(4)
C(10)-Fe(1)-C(9)-C(8)	-119.6(5)
C(6)-Fe(1)-C(9)-C(8)	-80.5(4)
C(7)-Fe(1)-C(9)-C(8)	-37.2(4)
C(8)-C(9)-C(10)-C(6)	-0.9(6)
Fe(1)-C(9)-C(10)-C(6)	-60.4(3)
C(8)-C(9)-C(10)-C(11)	176.2(5)
Fe(1)-C(9)-C(10)-C(11)	116.8(5)
C(8)-C(9)-C(10)-Fe(1)	59.4(4)
C(7)-C(6)-C(10)-C(9)	1.3(6)
Fe(1)-C(6)-C(10)-C(9)	61.0(3)
C(7)-C(6)-C(10)-C(11)	-175.8(5)
Fe(1)-C(6)-C(10)-C(11)	-116.2(4)
C(7)-C(6)-C(10)-Fe(1)	-59.6(4)
C(1)-Fe(1)-C(10)-C(9)	154.9(4)
C(2)-Fe(1)-C(10)-C(9)	-171.1(5)
C(5)-Fe(1)-C(10)-C(9)	110.7(4)
C(3)-Fe(1)-C(10)-C(9)	38.3(13)
C(4)-Fe(1)-C(10)-C(9)	70.0(4)
C(6)-Fe(1)-C(10)-C(9)	-117.3(4)
C(7)-Fe(1)-C(10)-C(9)	-80.3(4)
C(8)-Fe(1)-C(10)-C(9)	-37.4(4)
C(1)-Fe(1)-C(10)-C(6)	-87.8(4)
C(2)-Fe(1)-C(10)-C(6)	-53.8(6)

C(5)-Fe(1)-C(10)-C(6)	-132.0(3)
C(3)-Fe(1)-C(10)-C(6)	155.6(11)
C(4)-Fe(1)-C(10)-C(6)	-172.7(4)
C(7)-Fe(1)-C(10)-C(6)	37.0(3)
C(9)-Fe(1)-C(10)-C(6)	117.3(4)
C(8)-Fe(1)-C(10)-C(6)	80.0(3)
C(1)-Fe(1)-C(10)-C(11)	32.7(5)
C(2)-Fe(1)-C(10)-C(11)	66.7(6)
C(5)-Fe(1)-C(10)-C(11)	-11.5(5)
C(3)-Fe(1)-C(10)-C(11)	-83.9(13)
C(4)-Fe(1)-C(10)-C(11)	-52.2(5)
C(6)-Fe(1)-C(10)-C(11)	120.5(5)
C(7)-Fe(1)-C(10)-C(11)	157.5(4)
C(9)-Fe(1)-C(10)-C(11)	-122.2(5)
C(8)-Fe(1)-C(10)-C(11)	-159.5(4)
C(9)-C(10)-C(11)-N(1)	93.8(5)
C(6)-C(10)-C(11)-N(1)	-89.6(5)
Fe(1)-C(10)-C(11)-N(1)	-176.9(3)
C(12)-N(1)-C(11)-C(10)	-63.9(4)
C(14)-N(1)-C(11)-C(10)	-164.2(3)
C(11)-N(1)-C(12)-C(13)	-103.2(4)
C(14)-N(1)-C(12)-C(13)	12.2(3)
N(1)-C(12)-C(13)-C(14)	-12.1(3)
C(12)-N(1)-C(14)-C(15)	102.2(4)
C(11)-N(1)-C(14)-C(15)	-142.3(3)
C(12)-N(1)-C(14)-C(13)	-12.0(3)
C(11)-N(1)-C(14)-C(13)	103.5(4)
C(12)-C(13)-C(14)-N(1)	11.9(3)
C(12)-C(13)-C(14)-C(15)	-105.4(4)
N(1)-C(14)-C(15)-O(1)	-50.5(4)
C(13)-C(14)-C(15)-O(1)	49.4(4)
N(1)-C(14)-C(15)-C(22)	-165.9(3)
C(13)-C(14)-C(15)-C(22)	-66.0(4)
N(1)-C(14)-C(15)-C(16)	73.8(4)
C(13)-C(14)-C(15)-C(16)	173.7(3)
O(1)-C(15)-C(16)-C(17)	144.2(4)
C(22)-C(15)-C(16)-C(17)	-98.0(5)
C(14)-C(15)-C(16)-C(17)	20.5(5)
O(1)-C(15)-C(16)-C(21)	-38.9(5)
C(22)-C(15)-C(16)-C(21)	78.9(4)
C(14)-C(15)-C(16)-C(21)	-162.6(4)
C(21)-C(16)-C(17)-C(18)	-2.2(7)
C(15)-C(16)-C(17)-C(18)	174.7(5)
C(16)-C(17)-C(18)-C(19)	1.5(9)
C(17)-C(18)-C(19)-C(20)	0.0(9)
C(18)-C(19)-C(20)-C(21)	-0.7(8)
C(17)-C(16)-C(21)-C(20)	1.5(6)
C(15)-C(16)-C(21)-C(20)	-175.5(4)

C(19)-C(20)-C(21)-C(16)	-0.1(7)
O(1)-C(15)-C(22)-C(27)	5.3(5)
C(16)-C(15)-C(22)-C(27)	-114.2(4)
C(14)-C(15)-C(22)-C(27)	121.8(4)
O(1)-C(15)-C(22)-C(23)	-174.5(4)
C(16)-C(15)-C(22)-C(23)	66.0(5)
C(14)-C(15)-C(22)-C(23)	-58.0(5)
C(27)-C(22)-C(23)-C(24)	-0.7(7)
C(15)-C(22)-C(23)-C(24)	179.1(5)
C(22)-C(23)-C(24)-C(25)	2.0(8)
C(23)-C(24)-C(25)-C(26)	-1.7(9)
C(24)-C(25)-C(26)-C(27)	0.2(9)
C(23)-C(22)-C(27)-C(26)	-0.9(7)
C(15)-C(22)-C(27)-C(26)	179.3(5)
C(25)-C(26)-C(27)-C(22)	1.2(9)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for p1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5B)...O(3)#1	0.82	1.83	2.643(6)	168.2
O(1)-H(1E)...O(2)	0.87(6)	1.88(6)	2.734(5)	171(5)
N(1)-H(1F)...O(3)	0.89(5)	1.88(5)	2.731(4)	159(4)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z