Electronic Supplementary Material (ESI) for Analytical Methods.
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ha343 P -1 R = 0.04 : esday, 8 November 20

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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G TO T H E P A P E R

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C o n t e n t s
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Table S1 - Crystal Data and Details of the Structure Determination
for: ha343 P -1 R = 0.04

Crystal Data

Formula			C17 H14 N2 O4
Formula Weight			310.30
Crystal System			triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	7.8491(3)	8.9937(3)	11.0925(4)
alpha, beta, gamma [deg]	87.800(2)	87.763(2)	65.010(2)
V [Ang**3]			708.99(5)
Z			2
D(calc) [g/cm**3]			1.454
Mu(MoKa) [/mm]			0.105
F(000)			324
Crystal Size [mm]		0.15 x 0.42 x 0.46	

Data Collection

Temperature (K)			200
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			1.8, 28.3
Dataset		-10: 10 ; -11: 11 ; -14: 14	
Tot., Uniq. Data, R(int)		30194, 3530, 0.019	
Observed Data [I > 2.0 sigma(I)]			3011

Refinement

Nref, Npar			3530, 214
R, wR2, S		0.0366, 0.1090, 1.04	

w = ^2^(FO^2^)+(0.0586P)^2^+0.1635P] WHERE P=(FO^2^+2FC^2^)/3'

Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.21, 0.31

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: ha343 P -1 R = 0.04

Atom	x	y	z	U(eq) [Ang^2]
O1	0.65164(12)	0.06509(11)	0.52977(7)	0.0372(3)
O2	1.05773(12)	-0.05865(11)	0.35400(8)	0.0388(3)
O3	0.38078(12)	0.29913(13)	-0.07213(8)	0.0460(3)
O4	0.60226(10)	0.19548(10)	0.06293(7)	0.0287(2)
N1	0.29744(15)	0.43804(12)	0.41706(9)	0.0362(3)
N2	0.55225(13)	0.15244(12)	0.33922(8)	0.0290(3)
C1	0.54583(15)	0.16994(14)	0.45873(9)	0.0283(3)
C2	0.69559(15)	0.01497(13)	0.27608(10)	0.0293(3)
C3	0.94073(16)	0.39278(15)	-0.13892(10)	0.0318(3)
C11	0.39722(15)	0.32968(14)	0.50199(9)	0.0296(3)
C12	0.37030(18)	0.36033(16)	0.62466(10)	0.0369(3)
C13	0.2344(2)	0.51022(18)	0.66092(11)	0.0437(4)
C14	0.1312(2)	0.62245(17)	0.57424(13)	0.0467(4)
C15	0.1672(2)	0.58120(16)	0.45410(12)	0.0454(4)
C21	0.83192(14)	0.06702(12)	0.20723(9)	0.0250(3)
C22	1.01056(15)	0.03014(13)	0.24999(9)	0.0273(3)
C23	1.13261(14)	0.08431(13)	0.18676(10)	0.0290(3)
C24	1.07626(14)	0.17787(13)	0.08249(9)	0.0271(3)
C25	0.89638(14)	0.22014(12)	0.03700(9)	0.0238(3)
C26	0.82442(14)	0.32141(12)	-0.07006(9)	0.0256(3)
C27	0.65052(15)	0.35042(14)	-0.10625(9)	0.0298(3)
C28	0.53390(15)	0.28410(14)	-0.04280(10)	0.0311(3)
C29	0.78028(13)	0.16092(12)	0.10106(9)	0.0238(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: ha343 P -1 R = 0.04

Atom	x	y	z	U(iso) [Ang^2]
H2	0.470(2)	0.2386(18)	0.2967(13)	0.037(4)
H2A	0.63485	-0.02883	0.21931	0.0350
H2B	0.76480	-0.07359	0.33509	0.0350
H2C	1.15751	-0.05890	0.37898	0.0580
H3A	1.05391	0.30401	-0.17217	0.0480
H3B	0.97708	0.45747	-0.08483	0.0480
H3C	0.86749	0.46367	-0.20493	0.0480
H12	0.44360	0.28014	0.68229	0.0440
H13	0.21254	0.53531	0.74410	0.0520
H14	0.03696	0.72647	0.59654	0.0560
H15	0.09505	0.65931	0.39493	0.0540
H23	1.25479	0.05632	0.21602	0.0350
H24	1.15995	0.21445	0.04062	0.0320
H27	0.60344	0.41729	-0.17639	0.0360

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: ha343 P -1 R = 0.04

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.0367(4)	0.0452(5)	0.0317(4)	0.0137(3)	-0.0137(3)	-0.0194(4)
O2	0.0387(5)	0.0454(5)	0.0360(4)	0.0180(4)	-0.0170(4)	-0.0215(4)
O3	0.0322(4)	0.0724(7)	0.0387(5)	0.0176(4)	-0.0142(4)	-0.0276(4)
O4	0.0238(4)	0.0383(4)	0.0254(4)	0.0058(3)	-0.0050(3)	-0.0145(3)
N1	0.0464(6)	0.0334(5)	0.0265(5)	0.0034(4)	-0.0057(4)	-0.0145(4)
N2	0.0282(4)	0.0327(5)	0.0243(4)	0.0076(4)	-0.0036(3)	-0.0115(4)
C1	0.0281(5)	0.0369(6)	0.0256(5)	0.0080(4)	-0.0062(4)	-0.0196(4)
C2	0.0318(5)	0.0298(5)	0.0281(5)	0.0046(4)	-0.0036(4)	-0.0150(4)
C3	0.0357(6)	0.0390(6)	0.0245(5)	0.0046(4)	-0.0032(4)	-0.0196(5)
C11	0.0343(5)	0.0377(6)	0.0242(5)	0.0041(4)	-0.0042(4)	-0.0225(5)
C12	0.0447(6)	0.0492(7)	0.0249(5)	0.0030(5)	-0.0035(5)	-0.0279(6)
C13	0.0548(8)	0.0577(8)	0.0295(6)	-0.0094(5)	0.0049(5)	-0.0340(7)
C14	0.0552(8)	0.0410(7)	0.0443(7)	-0.0118(6)	0.0025(6)	-0.0202(6)
C15	0.0582(8)	0.0343(6)	0.0378(7)	0.0011(5)	-0.0080(6)	-0.0135(6)
C21	0.0266(5)	0.0247(5)	0.0233(5)	0.0005(4)	-0.0024(4)	-0.0105(4)
C22	0.0296(5)	0.0252(5)	0.0252(5)	0.0025(4)	-0.0066(4)	-0.0094(4)
C23	0.0237(5)	0.0319(5)	0.0304(5)	0.0003(4)	-0.0065(4)	-0.0105(4)
C24	0.0249(5)	0.0303(5)	0.0272(5)	-0.0011(4)	-0.0012(4)	-0.0126(4)
C25	0.0242(5)	0.0259(5)	0.0208(4)	-0.0015(4)	-0.0014(4)	-0.0099(4)
C26	0.0281(5)	0.0270(5)	0.0208(5)	-0.0020(4)	0.0000(4)	-0.0107(4)
C27	0.0307(5)	0.0350(6)	0.0227(5)	0.0049(4)	-0.0050(4)	-0.0130(4)
C28	0.0272(5)	0.0394(6)	0.0257(5)	0.0045(4)	-0.0061(4)	-0.0131(4)
C29	0.0217(4)	0.0259(5)	0.0226(5)	-0.0019(4)	-0.0029(3)	-0.0087(4)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and

h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: ha343 P -1 R = 0.04

O1	-C1	1.2379(14)	C22	-C23	1.4010(17)
O2	-C22	1.3486(14)	C23	-C24	1.3756(15)
O3	-C28	1.2077(17)	C24	-C25	1.4071(16)
O4	-C28	1.3837(14)	C25	-C26	1.4469(14)
O4	-C29	1.3773(14)	C25	-C29	1.3963(16)
N1	-C11	1.3390(15)	C26	-C27	1.3514(17)
N1	-C15	1.3294(17)	C27	-C28	1.4380(17)
N2	-C1	1.3375(13)	C2	-H2A	0.9900
N2	-C2	1.4542(15)	C2	-H2B	0.9900
O2	-H2C	0.8400	C3	-H3A	0.9800
C1	-C11	1.4994(16)	C3	-H3B	0.9800
N2	-H2	0.902(15)	C3	-H3C	0.9800
C2	-C21	1.5098(17)	C12	-H12	0.9500
C3	-C26	1.4940(17)	C13	-H13	0.9500
C11	-C12	1.3890(15)	C14	-H14	0.9500
C12	-C13	1.382(2)	C15	-H15	0.9500
C13	-C14	1.377(2)	C23	-H23	0.9500
C14	-C15	1.383(2)	C24	-H24	0.9500
C21	-C29	1.3915(14)	C27	-H27	0.9500
C21	-C22	1.3957(17)			

Table S6 - Bond Angles (Degrees)
for: ha343 P -1 R = 0.04

C28	-O4	-C29	121.60(9)	C3	-C26	-C25	120.37(10)
C11	-N1	-C15	117.26(10)	C3	-C26	-C27	120.76(10)
C1	-N2	-C2	123.95(10)	C25	-C26	-C27	118.87(10)
C22	-O2	-H2C	109.00	C26	-C27	-C28	122.62(10)
O1	-C1	-N2	124.09(11)	O4	-C28	-C27	117.12(11)
N2	-C1	-C11	114.37(10)	O3	-C28	-O4	116.46(11)
O1	-C1	-C11	121.54(9)	O3	-C28	-C27	126.41(11)
C2	-N2	-H2	119.7(9)	O4	-C29	-C21	115.28(10)
C1	-N2	-H2	115.9(9)	O4	-C29	-C25	121.17(9)
N2	-C2	-C21	110.94(9)	C21	-C29	-C25	123.54(10)
C1	-C11	-C12	120.14(10)	N2	-C2	-H2A	109.00
N1	-C11	-C12	123.22(11)	N2	-C2	-H2B	109.00
N1	-C11	-C1	116.64(9)	C21	-C2	-H2A	109.00
C11	-C12	-C13	118.45(11)	C21	-C2	-H2B	109.00
C12	-C13	-C14	118.75(12)	H2A	-C2	-H2B	108.00
C13	-C14	-C15	118.86(13)	C26	-C3	-H3A	109.00
N1	-C15	-C14	123.47(13)	C26	-C3	-H3B	109.00
C22	-C21	-C29	117.33(10)	C26	-C3	-H3C	109.00
C2	-C21	-C22	121.68(9)	H3A	-C3	-H3B	109.00
C2	-C21	-C29	120.93(10)	H3A	-C3	-H3C	109.00
O2	-C22	-C21	116.75(10)	H3B	-C3	-H3C	109.00
O2	-C22	-C23	122.48(11)	C11	-C12	-H12	121.00
C21	-C22	-C23	120.78(10)	C13	-C12	-H12	121.00
C22	-C23	-C24	120.28(11)	C12	-C13	-H13	121.00
C23	-C24	-C25	120.91(11)	C14	-C13	-H13	121.00
C26	-C25	-C29	118.44(10)	C13	-C14	-H14	121.00
C24	-C25	-C29	117.15(9)	C15	-C14	-H14	121.00
C24	-C25	-C26	124.41(10)	N1	-C15	-H15	118.00

Table S6 - Bond Angles (Degrees) (continued)
for: ha343 P -1 R = 0.04

C14	-C15	-H15	118.00	C25	-C24	-H24	120.00
C22	-C23	-H23	120.00	C26	-C27	-H27	119.00
C24	-C23	-H23	120.00	C28	-C27	-H27	119.00
C23	-C24	-H24	120.00				

Table S7 - Torsion Angles (Degrees)
for: ha343 P -1 R = 0.04

C29	-O4	-C28	-O3	175.56(10)
C29	-O4	-C28	-C27	-5.02(15)
C28	-O4	-C29	-C21	-178.32(9)
C28	-O4	-C29	-C25	2.79(15)
C15	-N1	-C11	-C1	-178.98(13)
C15	-N1	-C11	-C12	0.1(2)
C11	-N1	-C15	-C14	0.1(2)
C2	-N2	-C1	-O1	-6.1(2)
C2	-N2	-C1	-C11	174.02(11)
C1	-N2	-C2	-C21	-106.81(13)
O1	-C1	-C11	-N1	176.41(12)
O1	-C1	-C11	-C12	-2.7(2)
N2	-C1	-C11	-N1	-3.70(17)
N2	-C1	-C11	-C12	177.21(12)
N2	-C2	-C21	-C22	102.66(11)
N2	-C2	-C21	-C29	-74.21(12)
N1	-C11	-C12	-C13	-0.3(2)
C1	-C11	-C12	-C13	178.78(13)
C11	-C12	-C13	-C14	0.2(2)
C12	-C13	-C14	-C15	0.0(2)
C13	-C14	-C15	-N1	-0.2(3)
C2	-C21	-C22	-O2	1.97(15)
C2	-C21	-C22	-C23	-177.85(10)
C29	-C21	-C22	-O2	178.95(9)
C29	-C21	-C22	-C23	-0.87(15)
C2	-C21	-C29	-O4	-2.44(14)
C2	-C21	-C29	-C25	176.43(9)
C22	-C21	-C29	-O4	-179.44(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: ha343 P -1 R = 0.04

C22	-C21	-C29	-C25	-0.57(15)
O2	-C22	-C23	-C24	-178.47(10)
C21	-C22	-C23	-C24	1.34(16)
C22	-C23	-C24	-C25	-0.36(16)
C23	-C24	-C25	-C26	178.32(10)
C23	-C24	-C25	-C29	-1.00(15)
C24	-C25	-C26	-C3	-1.62(15)
C24	-C25	-C26	-C27	178.54(10)
C29	-C25	-C26	-C3	177.69(9)
C29	-C25	-C26	-C27	-2.15(14)
C24	-C25	-C29	-O4	-179.70(9)
C24	-C25	-C29	-C21	1.50(15)
C26	-C25	-C29	-O4	0.93(14)
C26	-C25	-C29	-C21	-177.86(9)
C3	-C26	-C27	-C28	179.93(12)
C25	-C26	-C27	-C28	-0.23(16)
C26	-C27	-C28	-O3	-176.87(12)
C26	-C27	-C28	-O4	3.77(16)

Table S8 - Contact Distances(Angstrom)
for: ha343 P -1 R = 0.04

O1	.C2	2.8516(14)	O3	.H3B_e	2.8800
O1	.C12	2.8485(16)	O3	.H12_f	2.7500
O1	.O2_b	2.6423(14)	O3	.H24_e	2.4500
O1	.C1_a	3.1014(16)	O3	.H27	2.6200
O1	.O1_a	3.1640(14)	O3	.H3A_e	2.8200
O2	.C15_c	3.1480(16)	O3	.H13_f	2.8100
O2	.O1_b	2.6423(14)	O4	.H2	2.735(15)
O2	.C2	2.7969(16)	O4	.H2A	2.5400
O3	.C24_e	3.4034(15)	N1	.H2	2.196(15)
O3	.C13_f	3.4181(16)	N1	.H3C_g	2.6700
O3	.C12_f	3.3857(14)	C1	.C21	3.4110(15)
O3	.C3_e	3.2988(17)	C1	.C1_a	3.5059(17)
O4	.C2	2.7565(14)	C1	.O1_a	3.1014(16)
O4	.N2	3.1048(12)	C2	.O4	2.7565(14)
O4	.C26	2.7999(14)	C2	.O1	2.8516(14)
O1	.H2B	2.4800	C2	.O2	2.7969(16)
O1	.H2C_b	1.8200	C3	.C24	3.0003(15)
N1	.N2	2.6530(14)	C3	.C13_j	3.583(2)
O1	.H12	2.5800	C3	.O3_i	3.2988(17)
N1	.C13	2.7825(16)	C11	.C14	2.7058(18)
N2	.O4	3.1048(12)	C12	.O3_l	3.3857(14)
O2	.H14_d	2.8300	C12	.C15	2.7089(18)
N2	.C29	3.1495(14)	C12	.O1	2.8485(16)
N2	.N1	2.6530(14)	C13	.C3_m	3.583(2)
N2	.C22	3.4048(17)	C13	.O3_l	3.4181(16)
O2	.H2B	2.3800	C13	.N1	2.7825(16)
O2	.H15_c	2.4500	C14	.C11	2.7058(18)
O2	.H23	2.6200	C14	.C15_n	3.559(2)

Table S8 - Contact Distances(Angstrom) (continued)
for: ha343 P -1 R = 0.04

C14	.C22_d	3.4875(18)	C1	.H12	2.6700
C15	.C14_n	3.559(2)	C1	.H2B	2.5500
C15	.O2_o	3.1480(16)	C2	.H3A_h	2.9600
C15	.C12	2.7089(18)	C3	.H3B_k	3.0800
C21	.C1	3.4110(15)	C3	.H15_g	2.9400
C21	.C24	2.8087(16)	C3	.H24	2.6800
C22	.C26_h	3.5327(14)	C3	.H27	2.6100
C22	.C14_d	3.4875(18)	C11	.H2	2.414(14)
C22	.C25	2.8047(14)	C15	.H3C_g	2.8500
C22	.N2	3.4048(17)	C21	.H2C	3.0400
C23	.C29	2.7516(16)	C21	.H2	2.762(16)
C24	.O3_i	3.4034(15)	C22	.H14_d	2.7200
C24	.C21	2.8087(16)	C22	.H2B	2.6100
C24	.C3	3.0003(15)	C23	.H2C	2.4200
C24	.C29_h	3.4779(14)	C23	.H14_d	2.9300
C25	.C22	2.8047(14)	C24	.H3A	2.9900
C25	.C28	2.8256(17)	C24	.H3B	2.9100
C26	.O4	2.7999(14)	C25	.H3B	2.7600
C26	.C22_h	3.5327(14)	C25	.H3A	2.8100
C27	.C28_g	3.4415(16)	C26	.H24	2.7200
C27	.C29	2.7650(14)	C27	.H3C	2.5200
C28	.C27_g	3.4415(16)	C27	.H3A	3.0800
C28	.C25	2.8256(17)	C29	.H2	3.065(16)
C29	.N2	3.1495(14)	C29	.H2A	2.7000
C29	.C27	2.7650(14)	H2	.O4	2.735(15)
C29	.C23	2.7516(16)	H2	.N1	2.196(15)
C29	.C24_h	3.4779(14)	H2	.C11	2.414(14)
C1	.H2C_b	2.8100	H2	.C21	2.762(16)

Table S8 - Contact Distances(Angstrom) (continued)
for: ha343 P -1 R = 0.04

H2	.C29	3.065(16)	H3C	.N1_g	2.6700
H2	.H2A	2.3700	H3C	.C15_g	2.8500
H2A	.O4	2.5400	H3C	.H15_g	2.3700
H2A	.C29	2.7000	H12	.O1	2.5800
H2A	.H2	2.3700	H12	.O3_l	2.7500
H2B	.O1	2.4800	H12	.C1	2.6700
H2B	.O2	2.3800	H12	.H13	2.3500
H2B	.C1	2.5500	H13	.O3_l	2.8100
H2B	.C22	2.6100	H13	.H12	2.3500
H2C	.C21	3.0400	H13	.H14	2.3400
H2C	.C23	2.4200	H14	.H13	2.3400
H2C	.H23	2.3100	H14	.H15	2.3200
H2C	.O1_b	1.8200	H14	.O2_d	2.8300
H2C	.C1_b	2.8100	H14	.C22_d	2.7200
H3A	.O3_i	2.8200	H14	.C23_d	2.9300
H3A	.C24	2.9900	H15	.O2_o	2.4500
H3A	.C25	2.8100	H15	.H14	2.3200
H3A	.C27	3.0800	H15	.C3_g	2.9400
H3A	.H24	2.5200	H15	.H3C_g	2.3700
H3A	.C2_h	2.9600	H23	.O2	2.6200
H3B	.O3_i	2.8800	H23	.H2C	2.3100
H3B	.C24	2.9100	H23	.H24	2.3200
H3B	.C25	2.7600	H24	.O3_i	2.4500
H3B	.H24	2.4600	H24	.C3	2.6800
H3B	.C3_k	3.0800	H24	.C26	2.7200
H3B	.H3B_k	2.1600	H24	.H3A	2.5200
H3C	.C27	2.5200	H24	.H3B	2.4600
H3C	.H27	2.2900	H24	.H23	2.3200

Table S8 - Contact Distances(Angstrom) (continued)
for: ha343 P -1 R = 0.04

H27	.O3	2.6200	H27	.H3C	2.2900
H27	.C3	2.6100			

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: ha343 P -1 R = 0.04

N2	-- H2	.. N1	0.902(15)	2.196(15)	2.6530(14)	110.7(11)	.
O2	-- H2C	.. O1	0.8400	1.8200	2.6423(14)	165.00	2_756
C2	-- H2B	.. O1	0.9900	2.4800	2.8516(14)	102.00	.
C2	-- H2B	.. O2	0.9900	2.3800	2.7969(16)	105.00	.
C15	-- H15	.. O2	0.9500	2.4500	3.1480(16)	130.00	1_465
C24	-- H24	.. O3	0.9500	2.4500	3.4034(15)	178.00	1_655

```
 Translation of Symmetry Code to Equiv.Pos


a =[  2656.00] = [   2_656] = 1-x,-y,1-z
b =[  2756.00] = [   2_756] = 2-x,-y,1-z
c =[  1645.00] = [   1_645] = 1+x,-1+y,z
d =[  2666.00] = [   2_666] = 1-x,1-y,1-z
e =[  1455.00] = [   1_455] = -1+x,y,z
f =[  1554.00] = [   1_554] = x,y,-1+z
g =[  2665.00] = [   2_665] = 1-x,1-y,-z
h =[  2755.00] = [   2_755] = 2-x,-y,-z
i =[  1655.00] = [   1_655] = 1+x,y,z
j =[  1654.00] = [   1_654] = 1+x,y,-1+z
k =[  2765.00] = [   2_765] = 2-x,1-y,-z
l =[  1556.00] = [   1_556] = x,y,1+z
m =[  1456.00] = [   1_456] = -1+x,y,1+z
n =[  2566.00] = [   2_566] = -x,1-y,1-z
o =[  1465.00] = [   1_465] = -1+x,1+y,z
_shelx_res_file
;
TITL ha343_a.res in P-1
    ha343.res
    created by SHELXL-2017/1 at 11:07:48 on 08-Nov-2017
REM Old TITL ha343_s_P-1 in P-1
REM SHELXT solution in P-1
REM R1 0.138,  Rweak 0.003,  Alpha 0.030,  Orientation as input
REM Formula found by SHELXT:  C17 N2 O4
CELL  0.71073   7.8491   8.9937  11.0925   87.800   87.763   65.010
ZERR    2.000   0.0003   0.0003   0.0004    0.002    0.002    0.002
LATT  1
SFAC C H N O
UNIT 34 28 4 8

EQIV $1  2-x,-y,1-z
EQIV $2  -1+x,1+y,z
EQIV $3  1+x,y,z

HTAB N2   N1
HTAB O2   O1_$1
HTAB C2   O1
HTAB C2   O2
HTAB C15  O2_$2
HTAB C24  O3_$3

ACTA NOHKL
BOND $H
CONF
FMAP 2
HTAB
L.S. 100
LIST 4
PLAN -20
SIZE 0.148 0.421 0.459
TEMP -73.150

REM WGHT 0.058600 0.163400
REM WGHT 0.058500 0.163900
REM WGHT 0.058600 0.163500
REM WGHT 0.058500 0.163900
WGHT    0.058600    0.163500
FVAR       0.27562
```

```
O1    4    0.651638    0.065090    0.529768    11.00000    0.03668    0.04519 =
         0.03166    0.01365   -0.01369   -0.01945
O2    4    1.057727   -0.058649    0.354002    11.00000    0.03871    0.04539 =
         0.03596    0.01798   -0.01705   -0.02146
AFIX 147
H2C   2    1.157510   -0.058901    0.378984    11.00000   -1.50000
AFIX   0
O3    4    0.380778    0.299129   -0.072134    11.00000    0.03225    0.07237 =
         0.03872    0.01757   -0.01418   -0.02760
O4    4    0.602260    0.195479    0.062929    11.00000    0.02383    0.03832 =
         0.02535    0.00581   -0.00501   -0.01445
N1    3    0.297439    0.438042    0.417057    11.00000    0.04636    0.03336 =
         0.02650    0.00343   -0.00574   -0.01450
N2    3    0.552252    0.152443    0.339223    11.00000    0.02825    0.03266 =
         0.02433    0.00756   -0.00362   -0.01147
C1    1    0.545825    0.169942    0.458728    11.00000    0.02812    0.03689 =
         0.02556    0.00799   -0.00623   -0.01962
C2    1    0.695586    0.014971    0.276079    11.00000    0.03175    0.02983 =
         0.02812    0.00456   -0.00361   -0.01495
AFIX  23
H2A   2    0.634855   -0.028826    0.219307    11.00000   -1.20000
H2B   2    0.764797   -0.073592    0.335087    11.00000   -1.20000
AFIX   0
C3    1    0.940727    0.392780   -0.138918    11.00000    0.03570    0.03899 =
         0.02454    0.00461   -0.00319   -0.01965
AFIX 137
H3A   2    1.053909    0.304014   -0.172171    11.00000   -1.50000
H3B   2    0.977079    0.457473   -0.084826    11.00000   -1.50000
H3C   2    0.867490    0.463669   -0.204926    11.00000   -1.50000
AFIX   0
C11   1    0.397221    0.329683    0.501993    11.00000    0.03431    0.03773 =
         0.02420    0.00407   -0.00417   -0.02253
C12   1    0.370296    0.360330    0.624658    11.00000    0.04473    0.04920 =
         0.02489    0.00304   -0.00347   -0.02794
AFIX  43
H12   2    0.443596    0.280138    0.682285    11.00000   -1.20000
AFIX   0
C13   1    0.234371    0.510218    0.660924    11.00000    0.05479    0.05765 =
         0.02953   -0.00940    0.00492   -0.03395
AFIX  43
H13   2    0.212540    0.535305    0.744101    11.00000   -1.20000
AFIX   0
C14   1    0.131238    0.622451    0.574243    11.00000    0.05525    0.04100 =
         0.04427   -0.01178    0.00248   -0.02021
AFIX  43
H14   2    0.036958    0.726466    0.596545    11.00000   -1.20000
AFIX   0
C15   1    0.167218    0.581200    0.454098    11.00000    0.05821    0.03434 =
         0.03784    0.00108   -0.00800   -0.01346
AFIX  43
H15   2    0.095051    0.659306    0.394930    11.00000   -1.20000
AFIX   0
C21   1    0.831922    0.067018    0.207233    11.00000    0.02663    0.02472 =
         0.02333    0.00050   -0.00235   -0.01054
C22   1    1.010561    0.030140    0.249986    11.00000    0.02955    0.02521 =
         0.02517    0.00251   -0.00664   -0.00937
C23   1    1.132610    0.084314    0.186759    11.00000    0.02367    0.03195 =
         0.03035    0.00030   -0.00650   -0.01053
AFIX  43
H23   2    1.254795    0.056322    0.216018    11.00000   -1.20000
AFIX   0
C24   1    1.076261    0.177868    0.082492    11.00000    0.02491    0.03029 =
         0.02715   -0.00110   -0.00118   -0.01262
AFIX  43
```

```
H24   2    1.159945    0.214449    0.040616    11.00000   -1.20000
AFIX   0
C25   1    0.896383    0.220139    0.036996    11.00000    0.02421    0.02595 =
         0.02084   -0.00150   -0.00141   -0.00990
C26   1    0.824416    0.321410   -0.070059    11.00000    0.02808    0.02696 =
         0.02083   -0.00197   -0.00001   -0.01071
C27   1    0.650518    0.350417   -0.106246    11.00000    0.03074    0.03505 =
         0.02271    0.00495   -0.00503   -0.01303
AFIX  43
H27   2    0.603438    0.417289   -0.176395    11.00000   -1.20000
AFIX   0
C28   1    0.533896    0.284099   -0.042804    11.00000    0.02723    0.03941 =
         0.02565    0.00453   -0.00609   -0.01311
C29   1    0.780285    0.160921    0.101062    11.00000    0.02167    0.02595 =
         0.02263   -0.00189   -0.00287   -0.00865
H2    2    0.469917    0.238575    0.296714    11.00000    0.03732
HKLF 4



REM  ha343_a.res in P-1
REM R1 =  0.0366 for    3011 Fo > 4sig(Fo)  and  0.0438 for all    3530 data
REM    214 parameters refined using      0 restraints

END

WGHT      0.0585      0.1639

REM Instructions for potential hydrogen bonds
HTAB O2 O1_$1
HTAB C15 O2_$2
HTAB N2 N1

REM Highest difference peak  0.310,  deepest hole -0.212,  1-sigma level  0.041
Q1    1   0.8437  0.1860  0.0631  11.00000  0.05    0.31
Q2    1   0.7708  0.0453  0.2379  11.00000  0.05    0.29
Q3    1   0.9257  0.0330  0.2206  11.00000  0.05    0.27
Q4    1   0.5999  0.3163 -0.0708  11.00000  0.05    0.26
Q5    1   0.4665  0.2554  0.4831  11.00000  0.05    0.26
Q6    1   1.0690  0.0643  0.2171  11.00000  0.05    0.25
Q7    1   0.8814  0.3589 -0.1002  11.00000  0.05    0.25
Q8    1   0.9100  0.0674  0.2336  11.00000  0.05    0.24
Q9    1   0.9803  0.2051  0.0618  11.00000  0.05    0.24
Q10   1   0.8592  0.2716 -0.0155  11.00000  0.05    0.23
Q11   1   0.3945  0.3485  0.5593  11.00000  0.05    0.23
Q12   1   0.5508  0.4697 -0.2024  11.00000  0.05    0.22
Q13   1   0.7275  0.3515 -0.0737  11.00000  0.05    0.22
Q14   1   0.7559  0.2982 -0.1042  11.00000  0.05    0.21
Q15   1   0.8083  0.1197  0.1607  11.00000  0.05    0.21
Q16   1   0.8227  0.0762  0.1442  11.00000  0.05    0.19
Q17   1   1.1123  0.0938  0.1220  11.00000  0.05    0.18
Q18   1   0.2812  0.4293  0.6404  11.00000  0.05    0.18
Q19   1   1.0396  0.3830 -0.1051  11.00000  0.05    0.16
Q20   1   0.1750  0.6100  0.5150  11.00000  0.05    0.15
;
_shelx_res_checksum                                99617
_iucr_refine_reflections_details
;
;

#===END
```