Table 1. Crystal data and structure refinement for shelxl.

Identification code	Tert-butyl-1, 1-dimethyl-3-oxo-2-oxa-5-azaspiro[3.4]octan-5-carboxylate (13)
Empirical formula	C13 H21 N O4
Formula weight	255.31
Temperature	150(2) K
Wavelength	0.71069 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 11.900(4) A alpha = 90 deg. b = 9.930(4) A beta = 110.21(3) deg. c = 12.406(5) A gamma = 90 deg.
Volume	1375.8(9) A^3
Z, Calculated density	4, 1.233 Mg/m^3
Absorption coefficient	0.091 mm^-1
F(000)	552
Crystal size	0.35 x 0.10 x 0.15 mm
Theta range for data collection	1.82 to 25.00 deg.
Limiting indices	0<=h<=14, 0<=k<=11, -14<=l<=13
Reflections collected / unique	2547 / 2425 [R(int) = 0.0487]
Completeness to theta = 25.00	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2425 / 0 / 169
Goodness-of-fit on F^2	0.978
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1184
R indices (all data)	R1 = 0.1468, wR2 = 0.1528
Extinction coefficient	0.007(2)
Largest diff. peak and hole	0.247 and -0.253 e.A^-3

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

	x	y	z	U(eq)
O(1)	1571(2)	4214(3)	6746(2)	33(1)
O(2)	604(2)	2438(3)	5644(2)	29(1)
O(3)	3473(2)	2042(2)	6748(2)	30(1)
O(4)	4871(2)	2482(2)	5920(2)	26(1)
N(1)	3000(2)	3142(3)	5044(2)	21(1)
C(1)	3374(3)	3801(4)	4155(3)	26(1)
C(2)	2193(3)	4330(4)	3328(3)	27(1)
C(3)	1468(3)	4606(3)	4099(3)	25(1)
C(4)	1753(3)	3376(3)	4883(2)	19(1)
C(5)	1391(3)	3475(4)	5940(3)	25(1)
C(6)	863(3)	2161(3)	4557(3)	24(1)
C(7)	1407(3)	783(3)	4589(3)	31(1)
C(8)	-286(3)	2326(4)	3547(3)	34(1)
C(9)	3770(3)	2510(3)	5982(3)	22(1)
C(10)	5843(3)	1692(3)	6748(3)	24(1)
C(11)	6831(3)	1802(4)	6246(3)	31(1)
C(12)	6221(3)	2339(4)	7926(3)	31(1)
C(13)	5471(3)	240(4)	6782(3)	35(1)

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

O(1)-C(5)	1.199(4)
O(2)-C(5)	1.355(4)
O(2)-C(6)	1.509(4)
O(3)-C(9)	1.215(4)
O(4)-C(9)	1.340(4)
O(4)-C(10)	1.478(4)
N(1)-C(9)	1.360(4)
N(1)-C(4)	1.446(4)
N(1)-C(1)	1.477(4)
C(1)-C(2)	1.519(5)
C(2)-C(3)	1.519(5)
C(3)-C(4)	1.525(4)
C(4)-C(5)	1.518(4)
C(4)-C(6)	1.563(4)
C(6)-C(7)	1.509(5)
C(6)-C(8)	1.511(4)
C(10)-C(11)	1.512(5)
C(10)-C(13)	1.513(5)
C(10)-C(12)	1.516(4)
C(5)-O(2)-C(6)	92.6(2)
C(9)-O(4)-C(10)	121.2(2)
C(9)-N(1)-C(4)	123.2(2)
C(9)-N(1)-C(1)	123.8(3)
C(4)-N(1)-C(1)	112.7(2)
N(1)-C(1)-C(2)	102.1(3)
C(3)-C(2)-C(1)	103.4(3)

C(2)-C(3)-C(4)	102.0(3)
N(1)-C(4)-C(5)	118.3(2)
N(1)-C(4)-C(3)	102.0(3)
C(5)-C(4)-C(3)	115.6(3)
N(1)-C(4)-C(6)	118.9(3)
C(5)-C(4)-C(6)	84.5(2)
C(3)-C(4)-C(6)	118.1(3)
O(1)-C(5)-O(2)	126.8(3)
O(1)-C(5)-C(4)	137.6(3)
O(2)-C(5)-C(4)	95.3(3)
O(2)-C(6)-C(7)	111.1(3)
O(2)-C(6)-C(8)	108.4(3)
C(7)-C(6)-C(8)	112.2(3)
O(2)-C(6)-C(4)	87.6(2)
C(7)-C(6)-C(4)	116.6(3)
C(8)-C(6)-C(4)	118.0(3)
O(3)-C(9)-O(4)	126.3(3)
O(3)-C(9)-N(1)	123.7(3)
O(4)-C(9)-N(1)	110.1(3)
O(4)-C(10)-C(11)	102.0(2)
O(4)-C(10)-C(13)	111.0(3)
C(11)-C(10)-C(13)	110.9(3)
O(4)-C(10)-C(12)	110.2(3)
C(11)-C(10)-C(12)	110.6(3)
C(13)-C(10)-C(12)	111.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for shelxl. 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
O(1)	34(2)	40(2)	24(1)	-12(1)	11(1)	1(1)
O(2)	29(1)	34(2)	28(1)	-3(1)	15(1)	-2(1)
O(3)	28(1)	38(2)	23(1)	11(1)	9(1)	4(1)
O(4)	19(1)	30(1)	28(1)	10(1)	7(1)	6(1)
N(1)	22(2)	27(2)	16(1)	5(1)	9(1)	3(1)
C(1)	24(2)	31(2)	27(2)	6(2)	13(1)	3(2)
C(2)	30(2)	26(2)	23(2)	3(2)	7(2)	-1(2)
C(3)	27(2)	21(2)	24(2)	2(2)	4(2)	3(2)
C(4)	20(2)	21(2)	16(2)	-2(1)	4(1)	-2(1)
C(5)	15(2)	33(2)	23(2)	0(2)	2(1)	3(2)
C(6)	27(2)	24(2)	23(2)	-1(2)	13(1)	1(2)
C(7)	36(2)	20(2)	39(2)	-4(2)	16(2)	-2(2)
C(8)	29(2)	33(2)	33(2)	-7(2)	2(2)	-3(2)
C(9)	24(2)	19(2)	21(2)	1(2)	7(1)	2(2)
C(10)	20(2)	20(2)	29(2)	2(2)	5(2)	2(2)
C(11)	24(2)	33(2)	34(2)	-4(2)	10(2)	6(2)
C(12)	27(2)	37(2)	26(2)	-3(2)	7(2)	2(2)
C(13)	33(2)	29(2)	39(2)	4(2)	6(2)	-2(2)