138472

LOK1388_1

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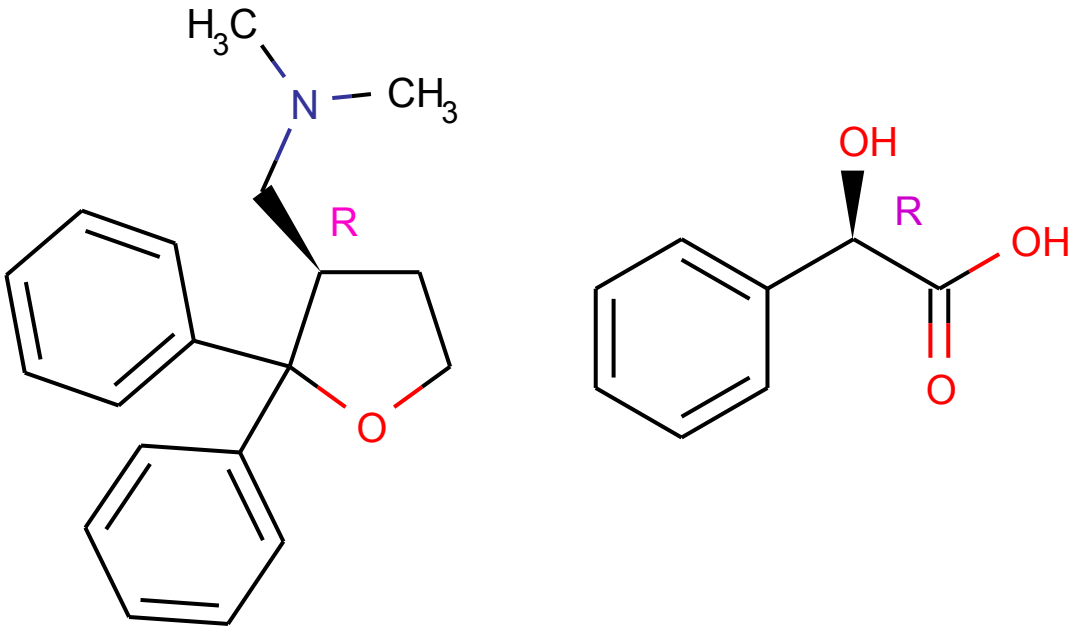
X-ray Structure Report



April 13, 2022

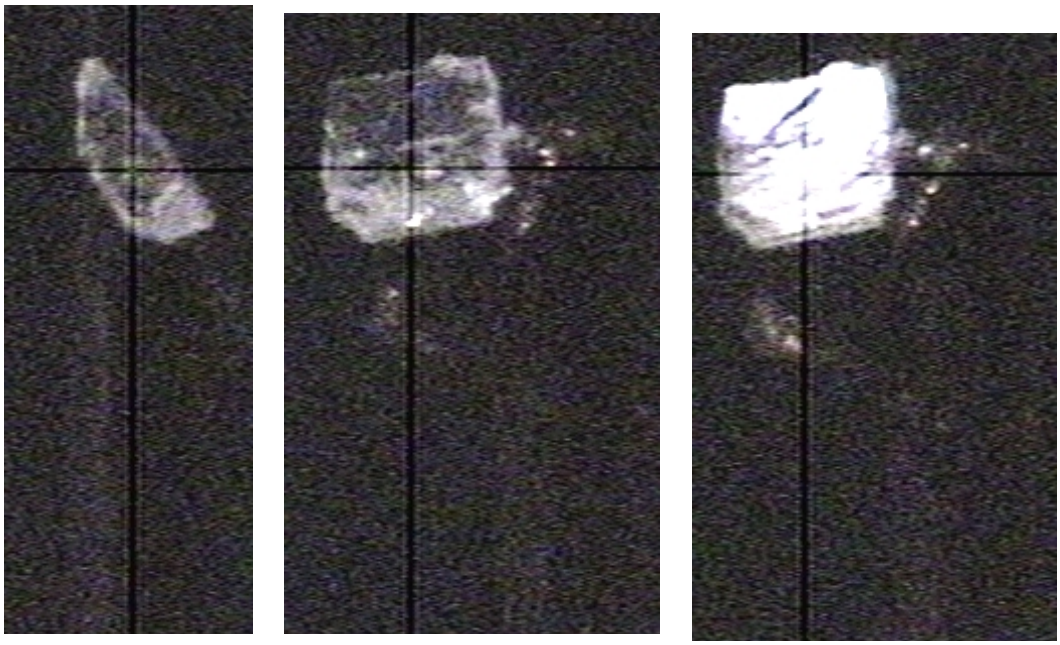


Fig. 1. The crystal

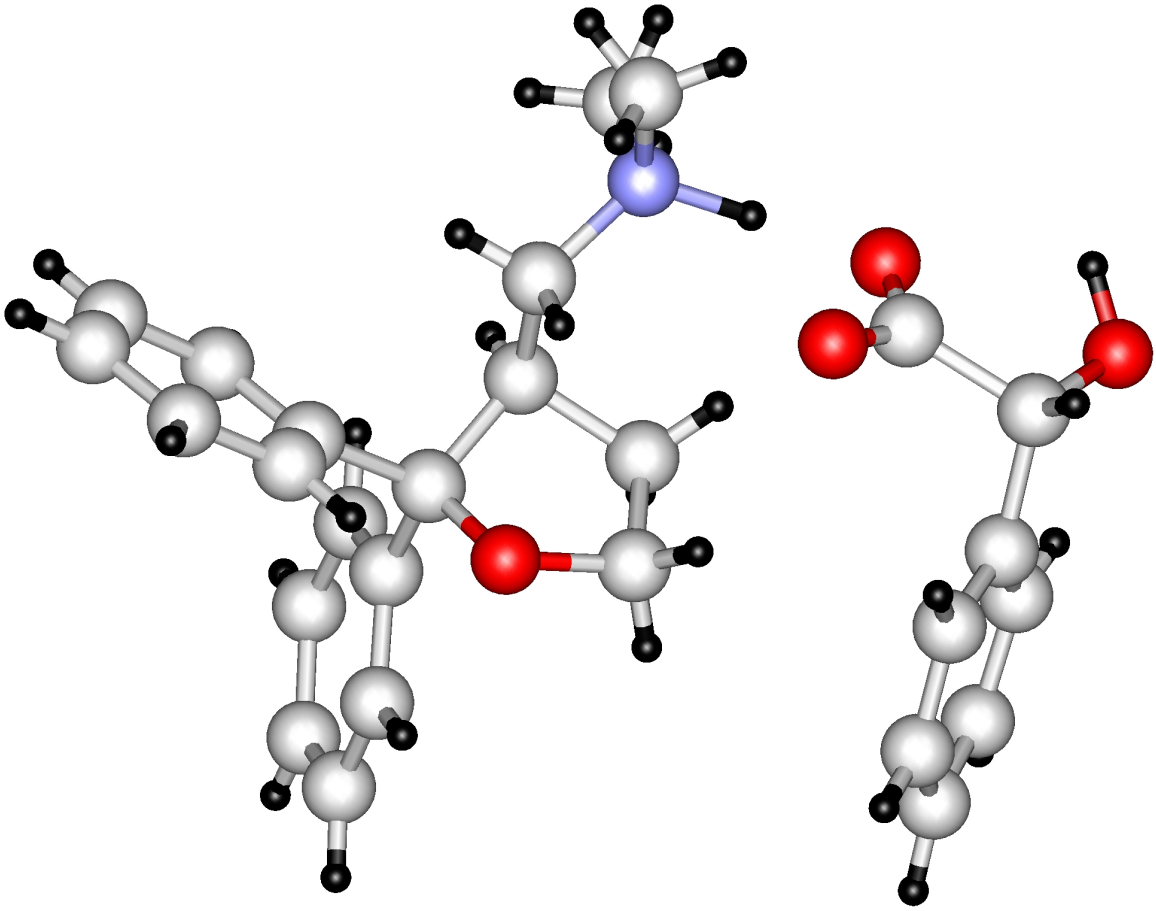


Fig. 2. The molecule (hydrogens were generated by the software)

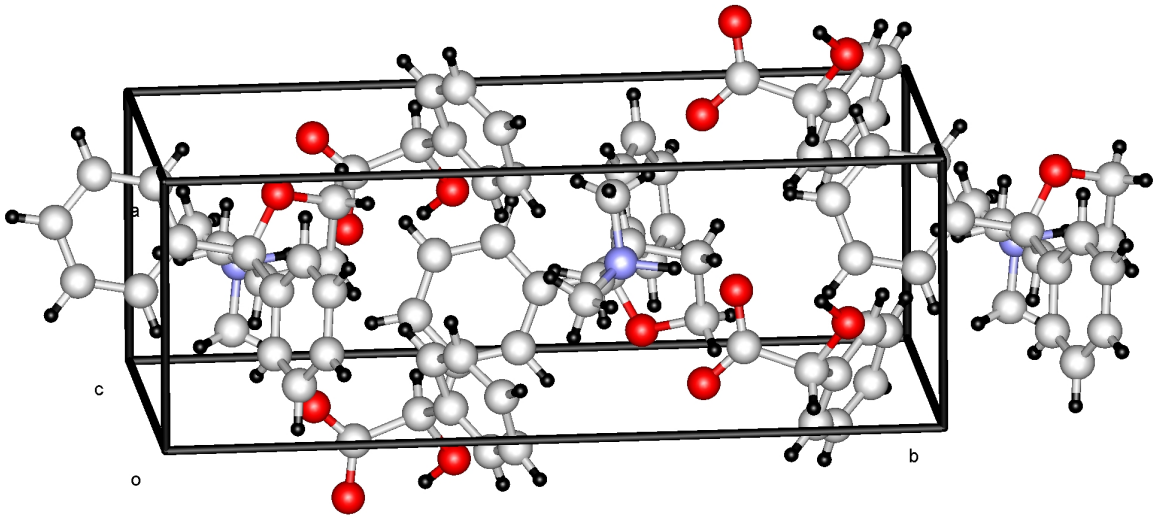


Fig. 3. Packing

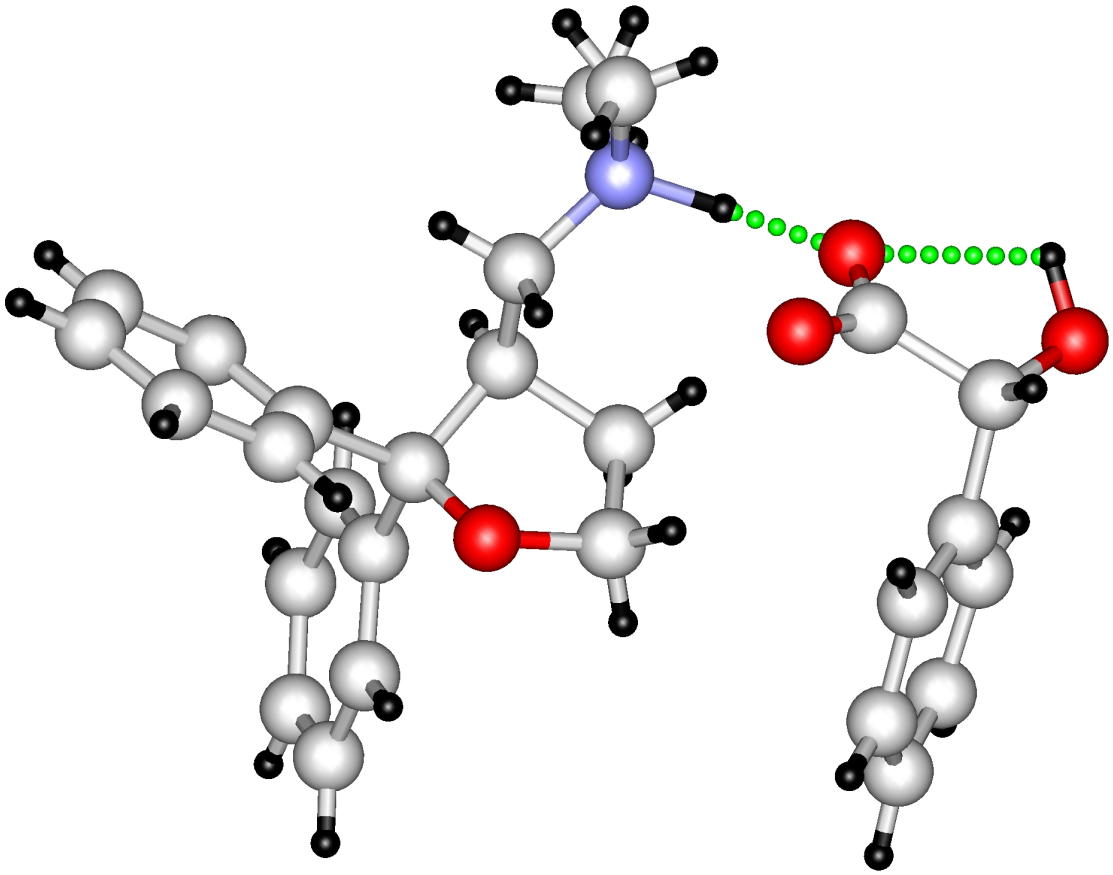


Fig. 3. Hydrogen bonds

Experimental

Data Collection

A colorless block crystal of $C_{27}H_{31}NO_4$ having approximate dimensions of 0.26 x 0.18 x 0.10 mm was mounted on a cactus needle. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Cu-Kα radiation.

Indexing was performed from 4 oscillations that were exposed for 60 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 6.2318(4) Å

b = 16.9732(9) Å β = 100.264(4)^o

c = 11.3789(7) Å

V = 1184.33(12) Å^3

For Z = 2 and F.W. = 433.55, the calculated density is 1.216 g/cm^3. Based on the systematic absences of:

0k0: k ± 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$P2_1$ (#4)

The data were collected at a temperature of 20 ± 1^{o}C to a maximum 2θ value of 143.5^o. A total of 180 oscillation images were collected. A sweep of data was done using ω scans from 20.0 to 200.0^o in 5.0^o step, at χ=0.0^o and ϕ = 0.0^o. The exposure rate was 36.0 [sec./^{o}]. A second sweep was performed using ω scans from 20.0 to 200.0^o in 5.0^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 36.0 [sec./^{o}]. Another sweep was performed using ω scans from 20.0 to 200.0^o in 5.0^o step, at χ=54.0^o and ϕ = 90.0^o. The exposure rate was 36.0 [sec./^{o}]. Another sweep was performed using ω scans from 20.0 to 200.0^o in 5.0^o step, at χ=54.0^o and ϕ = 180.0^o. The exposure rate was 36.0 [sec./^{o}]. Another sweep was performed using ω scans from 20.0 to 200.0^o in 5.0^o step, at χ=54.0^o and ϕ = 270.0^o. The exposure rate was 36.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 13708 reflections that were collected, 4116 were unique (R_{int} = 0.081).

The linear absorption coefficient, μ, for Cu-Kα radiation is 6.491 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.697 to 0.937. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction[1] was applied (coefficient = 11.366000).

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model.The final cycle of full-matrix least-squares refinement[4] on F was based on 6669 observed reflections ($I > 2.00\sigma(I)$) and 325 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0463$$

$$R_W = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.0545$$

The standard deviation of an observation of unit weight[5] was 5.78. Unit weights were used. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.90 and -1.77 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter 0.0(3).[6]

Neutral atom scattering factors were taken from Cromer and Waber[7]. Anomalous dispersion effects were included in Fcalc[8]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[9]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[10]. All calculations were performed using the CrystalStructure[11,12] crystallographic software package.

References

(1) Larson, A.C. (1970), Crystallographic Computing, 291-294. F.R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized:

$$\Sigma w(|F_o|-|F_c|)^2 \quad \text{where w = Least Squares weights.}$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

(7) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(8) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(9) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(10) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(11) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(12) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{31}NO_4$
Formula Weight	433.55
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.26 X 0.18 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	4 oscillations @ 60.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 6.2318(4) Å b = 16.9732(9) Å c = 11.3789(7) Å β = 100.264(4) ^{o} V = 1184.33(12) Å^3
Space Group	$P2_1$ (#4)
Z value	2
D_{calc}	1.216 g/cm^3
F_{000}	464.00
μ(CuKα)	6.491 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	CuKα (λ = 1.54187 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	180 exposures
ω oscillation Range (χ=0.0, ϕ=0.0)	20.0 - 200.0°
Exposure Rate	36.0 sec./°
ω oscillation Range (χ=54.0, ϕ=0.0)	20.0 - 200.0°
Exposure Rate	36.0 sec./°
ω oscillation Range (χ=54.0, ϕ=90.0)	20.0 - 200.0°
Exposure Rate	36.0 sec./°
ω oscillation Range (χ=54.0, ϕ=180.0)	20.0 - 200.0°
Exposure Rate	36.0 sec./°
ω oscillation Range (χ=54.0, ϕ=270.0)	20.0 - 200.0°
Exposure Rate	36.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	143.5°
No. of Reflections Measured	Total: 13708 Unique: 4116 (R_{int} = 0.081) Friedel pairs: 1760
Corrections	Lorentz-polarization Absorption (trans. factors: 0.697 - 0.937) Secondary Extinction (coefficient: 1.13660e+001)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1
$2\theta_{max}$ cutoff	143.5^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	6669
No. Variables	325
Reflection/Parameter Ratio	20.52
Residuals: R (I>2.00σ(I))	0.0463
Residuals: Rw (I>2.00σ(I))	0.0545
Goodness of Fit Indicator	5.784
Flack Parameter	0.0(3)
Max Shift/Error in Final Cycle	0.007
Maximum peak in Final Diff. Map	1.90 e$^-$/Å^3
Minimum peak in Final Diff. Map	-1.77 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O(1)	0.8950(5)	0.1524(2)	0.1425(2)	4.14(10)
O(2)	0.6342(8)	0.2575(2)	0.5047(3)	5.55(13)
O(4)	0.9738(7)	0.2146(2)	0.5133(3)	6.23(13)
O(5)	0.7410(7)	0.3975(2)	0.5822(3)	7.60(14)
N(1)	0.5473(8)	0.1136(3)	0.4200(3)	3.70(13)
C(1)	0.8387(13)	0.2663(4)	0.5218(4)	4.3(2)
C(6)	0.6924(9)	0.1128(3)	0.1018(4)	3.36(15)
C(7)	0.6425(8)	0.0880(2)	0.3145(4)	3.79(16)
C(8)	0.5901(9)	0.1427(3)	-0.0211(4)	3.42(15)
C(9)	0.5579(8)	0.1336(2)	0.1977(4)	3.15(14)
C(11)	0.7439(10)	0.0240(3)	0.0948(4)	3.40(16)
C(12)	0.3071(9)	0.1043(3)	0.3991(4)	6.3(2)
C(13)	0.9804(12)	0.3865(3)	0.4327(6)	4.34(18)
C(14)	0.6459(8)	0.0630(3)	0.5229(4)	5.04(16)
C(15)	0.3707(9)	0.1374(3)	-0.0667(4)	4.42(16)
C(16)	0.4272(11)	0.1962(3)	-0.2504(5)	5.11(19)
C(17)	0.5779(9)	-0.0287(4)	0.0581(4)	5.2(2)
C(18)	0.8332(15)	-0.1367(4)	0.0848(6)	6.9(2)
C(19)	1.088(2)	0.4427(5)	0.2228(7)	9.4(3)
C(20)	1.1722(12)	0.3635(3)	0.4014(7)	6.4(2)
C(21)	0.2892(9)	0.1640(3)	-0.1812(5)	5.10(18)
C(22)	0.8387(11)	0.4343(4)	0.3600(7)	5.9(2)
C(23)	0.6073(10)	0.2213(3)	0.2104(4)	4.99(18)
C(24)	0.7221(9)	0.1743(3)	-0.0944(4)	5.49(18)
C(25)	0.8424(10)	0.2276(3)	0.1884(5)	5.8(2)
C(26)	0.6224(13)	-0.1094(4)	0.0551(5)	6.6(2)
C(27)	0.9523(9)	-0.0056(3)	0.1260(4)	4.63(19)
C(28)	0.9965(12)	-0.0843(4)	0.1210(6)	6.5(2)
C(29)	0.6445(11)	0.2024(3)	-0.2071(5)	6.2(2)
C(30)	1.2183(13)	0.3931(5)	0.2966(9)	7.9(3)
C(31)	0.9231(11)	0.3518(3)	0.5478(5)	5.5(2)
C(32)	0.8864(16)	0.4607(5)	0.2518(7)	8.4(3)
H(1)	0.564(9)	0.180(4)	0.452(4)	8.8(17)
H(2)	0.2743	0.1165	-0.0187	5.31
H(3)	0.3729	0.2146	-0.3289	6.15
H(4)	0.4333	-0.0093	0.0363	6.28
H(5)	0.8591	-0.1917	0.0819	8.82

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(6)	1.1312	0.4633	0.1531	11.25
H(7)	1.2706	0.3296	0.4511	7.75
H(8)	0.1381	0.1600	-0.2135	6.04
H(9)	0.7075	0.4507	0.3842	6.97
H(10)	0.8733	0.1781	-0.0623	6.57
H(11)	0.5058	-0.1451	0.0305	8.13
H(12)	1.0688	0.0303	0.1498	5.47
H(13)	1.1411	-0.1040	0.1412	7.97
H(14)	0.7426	0.2245	-0.2531	7.53
H(15)	1.3529	0.3801	0.2731	10.10
H(16)	0.7848	0.4896	0.1959	9.90
H(17)	0.4074	0.1233	0.1707	3.81
H(18)	0.7960	0.0951	0.3330	4.68
H(19)	0.6106	0.0337	0.3004	4.67
H(20)	0.5111	0.2499	0.1513	5.95
H(21)	0.5938	0.2400	0.2874	5.97
H(22)	0.9365	0.2402	0.2612	6.88
H(23)	0.8532	0.2673	0.1308	6.89
H(26)	0.6479	0.3617	0.6130	9.34
H(27)	0.2425	0.1512	0.3634	7.73
H(28)	0.2602	0.0958	0.4731	7.72
H(29)	0.2644	0.0610	0.3475	7.72
H(30)	0.5583	0.0174	0.5253	6.14
H(31)	0.6525	0.0920	0.5949	6.16
H(32)	0.7888	0.0476	0.5142	6.16
H(33)	1.0452	0.3512	0.6110	6.28

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.051(2)	0.056(3)	0.048(2)	-0.014(2)	0.003(2)	-0.006(2)
O(2)	0.074(3)	0.060(3)	0.071(3)	0.003(3)	-0.004(2)	-0.001(2)
O(4)	0.088(3)	0.056(3)	0.093(3)	0.017(2)	0.017(2)	0.005(2)
O(5)	0.136(4)	0.072(3)	0.087(3)	0.007(3)	0.038(3)	-0.010(2)
N(1)	0.059(3)	0.048(3)	0.037(2)	0.012(3)	0.019(2)	0.007(2)
C(1)	0.082(6)	0.051(5)	0.026(3)	-0.002(5)	-0.001(3)	0.004(3)
C(6)	0.052(4)	0.040(4)	0.038(3)	-0.014(3)	0.013(3)	-0.006(3)
C(7)	0.047(3)	0.049(4)	0.052(3)	0.006(3)	0.020(3)	-0.005(3)
C(8)	0.046(3)	0.049(4)	0.035(3)	0.005(3)	0.009(3)	0.003(3)
C(9)	0.056(4)	0.027(3)	0.038(3)	0.006(3)	0.012(3)	0.002(2)
C(11)	0.041(4)	0.058(4)	0.032(3)	-0.002(3)	0.010(3)	-0.004(3)
C(12)	0.068(5)	0.096(5)	0.080(5)	0.001(4)	0.026(3)	0.002(3)
C(13)	0.066(5)	0.036(4)	0.059(4)	-0.006(4)	0.001(4)	-0.014(3)
C(14)	0.095(4)	0.054(4)	0.045(3)	0.020(4)	0.020(3)	0.017(3)
C(15)	0.058(4)	0.064(4)	0.046(3)	0.013(3)	0.012(3)	0.007(3)
C(16)	0.087(5)	0.071(5)	0.036(3)	0.022(4)	0.013(4)	-0.002(3)
C(17)	0.054(4)	0.060(5)	0.084(4)	0.003(4)	0.015(3)	-0.017(3)
C(18)	0.144(8)	0.040(6)	0.095(6)	0.026(5)	0.064(6)	0.010(4)
C(19)	0.190(11)	0.081(7)	0.086(6)	-0.047(7)	0.023(8)	0.022(5)
C(20)	0.067(5)	0.063(5)	0.114(7)	-0.004(4)	0.021(5)	-0.019(5)
C(21)	0.050(4)	0.089(5)	0.052(3)	0.010(4)	0.002(3)	-0.004(4)
C(22)	0.076(6)	0.066(5)	0.079(5)	0.014(4)	0.006(4)	0.004(4)
C(23)	0.105(5)	0.051(4)	0.033(3)	0.014(4)	0.010(3)	0.003(3)
C(24)	0.067(5)	0.098(5)	0.043(3)	0.009(4)	0.009(3)	0.011(4)
C(25)	0.119(6)	0.040(4)	0.059(4)	-0.027(4)	0.009(4)	-0.001(3)
C(26)	0.107(6)	0.043(5)	0.107(6)	-0.017(4)	0.042(5)	-0.018(4)
C(27)	0.056(5)	0.052(4)	0.065(4)	0.002(4)	0.004(3)	-0.007(3)
C(28)	0.080(6)	0.066(6)	0.106(6)	0.013(5)	0.030(5)	0.006(4)
C(29)	0.075(5)	0.116(6)	0.048(4)	-0.005(5)	0.019(4)	0.026(4)
C(30)	0.113(7)	0.085(6)	0.122(8)	-0.035(5)	0.074(6)	-0.056(5)
C(31)	0.105(6)	0.041(4)	0.052(4)	0.001(4)	-0.015(4)	-0.009(3)
C(32)	0.115(7)	0.105(7)	0.094(7)	0.010(6)	0.002(6)	0.012(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O(1)	C(6)	1.433(6)	O(1)	C(25)	1.439(7)
O(2)	C(1)	1.263(9)	O(4)	C(1)	1.232(8)
O(5)	C(31)	1.484(8)	O(5)	H(26)	0.950
N(1)	C(7)	1.496(7)	N(1)	C(12)	1.482(7)
N(1)	C(14)	1.493(6)	N(1)	H(1)	1.19(7)
C(1)	C(31)	1.554(9)	C(6)	C(8)	1.517(7)
C(6)	C(9)	1.531(8)	C(6)	C(11)	1.547(8)
C(7)	C(9)	1.547(6)	C(7)	H(18)	0.950
C(7)	H(19)	0.950	C(8)	C(15)	1.376(8)
C(8)	C(24)	1.381(8)	C(9)	C(23)	1.521(7)
C(9)	H(17)	0.950	C(11)	C(17)	1.374(8)
C(11)	C(27)	1.379(8)	C(12)	H(27)	0.950
C(12)	H(28)	0.950	C(12)	H(29)	0.950
C(13)	C(20)	1.364(11)	C(13)	C(22)	1.365(9)
C(13)	C(31)	1.535(9)	C(14)	H(30)	0.950
C(14)	H(31)	0.950	C(14)	H(32)	0.950
C(15)	C(21)	1.387(7)	C(15)	H(2)	0.950
C(16)	C(21)	1.378(9)	C(16)	C(29)	1.360(9)
C(16)	H(3)	0.950	C(17)	C(26)	1.399(10)
C(17)	H(4)	0.950	C(18)	C(26)	1.377(11)
C(18)	C(28)	1.358(11)	C(18)	H(5)	0.950
C(19)	C(30)	1.353(12)	C(19)	C(32)	1.387(16)
C(19)	H(6)	0.950	C(20)	C(30)	1.372(13)
C(20)	H(7)	0.950	C(21)	H(8)	0.950
C(22)	C(32)	1.391(12)	C(22)	H(9)	0.950
C(23)	C(25)	1.533(9)	C(23)	H(20)	0.950
C(23)	H(21)	0.950	C(24)	C(29)	1.373(8)
C(24)	H(10)	0.950	C(25)	H(22)	0.950
C(25)	H(23)	0.950	C(26)	H(11)	0.950
C(27)	C(28)	1.367(10)	C(27)	H(12)	0.950
C(28)	H(13)	0.950	C(29)	H(14)	0.950
C(30)	H(15)	0.950	C(31)	H(33)	0.950
C(32)	H(16)	0.950			

Table 4. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	O(1)	C(25)	106.8(4)	C(31)	O(5)	H(26)	108.0
C(7)	N(1)	C(12)	111.9(3)	C(7)	N(1)	C(14)	107.2(4)
C(7)	N(1)	H(1)	120(2)	C(12)	N(1)	C(14)	109.1(4)
C(12)	N(1)	H(1)	100(2)	C(14)	N(1)	H(1)	108(2)
O(2)	C(1)	O(4)	126.1(6)	O(2)	C(1)	C(31)	115.9(6)
O(4)	C(1)	C(31)	117.9(6)	O(1)	C(6)	C(8)	110.0(4)
O(1)	C(6)	C(9)	103.0(3)	O(1)	C(6)	C(11)	107.2(4)
C(8)	C(6)	C(9)	112.7(4)	C(8)	C(6)	C(11)	109.6(4)
C(9)	C(6)	C(11)	114.0(4)	N(1)	C(7)	C(9)	114.9(4)
N(1)	C(7)	H(18)	108.2	N(1)	C(7)	H(19)	108.4
C(9)	C(7)	H(18)	107.6	C(9)	C(7)	H(19)	108.2
H(18)	C(7)	H(19)	109.5	C(6)	C(8)	C(15)	123.5(5)
C(6)	C(8)	C(24)	119.3(5)	C(15)	C(8)	C(24)	117.1(4)
C(6)	C(9)	C(7)	110.5(4)	C(6)	C(9)	C(23)	99.6(4)
C(6)	C(9)	H(17)	111.2	C(7)	C(9)	C(23)	112.1(3)
C(7)	C(9)	H(17)	110.6	C(23)	C(9)	H(17)	112.5
C(6)	C(11)	C(17)	119.9(5)	C(6)	C(11)	C(27)	122.5(5)
C(17)	C(11)	C(27)	117.7(5)	N(1)	C(12)	H(27)	108.6
N(1)	C(12)	H(28)	109.6	N(1)	C(12)	H(29)	110.2
H(27)	C(12)	H(28)	109.5	H(27)	C(12)	H(29)	109.5
H(28)	C(12)	H(29)	109.5	C(20)	C(13)	C(22)	121.0(7)
C(20)	C(13)	C(31)	117.4(6)	C(22)	C(13)	C(31)	121.5(7)
N(1)	C(14)	H(30)	109.5	N(1)	C(14)	H(31)	109.1
N(1)	C(14)	H(32)	109.9	H(30)	C(14)	H(31)	109.5
H(30)	C(14)	H(32)	109.5	H(31)	C(14)	H(32)	109.5
C(8)	C(15)	C(21)	120.4(5)	C(8)	C(15)	H(2)	119.7
C(21)	C(15)	H(2)	119.9	C(21)	C(16)	C(29)	120.4(5)
C(21)	C(16)	H(3)	120.9	C(29)	C(16)	H(3)	118.7
C(11)	C(17)	C(26)	120.1(5)	C(11)	C(17)	H(4)	118.8
C(26)	C(17)	H(4)	121.1	C(26)	C(18)	C(28)	119.0(7)
C(26)	C(18)	H(5)	118.9	C(28)	C(18)	H(5)	122.1
C(30)	C(19)	C(32)	117.3(9)	C(30)	C(19)	H(6)	121.2
C(32)	C(19)	H(6)	121.4	C(13)	C(20)	C(30)	116.8(6)
C(13)	C(20)	H(7)	121.4	C(30)	C(20)	H(7)	121.8
C(15)	C(21)	C(16)	120.3(5)	C(15)	C(21)	H(8)	120.8
C(16)	C(21)	H(8)	119.0	C(13)	C(22)	C(32)	120.7(7)
C(13)	C(22)	H(9)	119.7	C(32)	C(22)	H(9)	119.5

Table 4. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(9)	C(23)	C(25)	103.7(4)	C(9)	C(23)	H(20)	109.9
C(9)	C(23)	H(21)	111.4	C(25)	C(23)	H(20)	110.5
C(25)	C(23)	H(21)	111.8	H(20)	C(23)	H(21)	109.5
C(8)	C(24)	C(29)	123.4(5)	C(8)	C(24)	H(10)	116.8
C(29)	C(24)	H(10)	119.8	O(1)	C(25)	C(23)	106.5(4)
O(1)	C(25)	H(22)	111.7	O(1)	C(25)	H(23)	109.2
C(23)	C(25)	H(22)	109.5	C(23)	C(25)	H(23)	110.5
H(22)	C(25)	H(23)	109.5	C(17)	C(26)	C(18)	120.6(6)
C(17)	C(26)	H(11)	119.2	C(18)	C(26)	H(11)	120.2
C(11)	C(27)	C(28)	122.2(5)	C(11)	C(27)	H(12)	118.5
C(28)	C(27)	H(12)	119.3	C(18)	C(28)	C(27)	120.4(6)
C(18)	C(28)	H(13)	118.1	C(27)	C(28)	H(13)	121.5
C(16)	C(29)	C(24)	118.3(6)	C(16)	C(29)	H(14)	121.8
C(24)	C(29)	H(14)	119.8	C(19)	C(30)	C(20)	124.9(9)
C(19)	C(30)	H(15)	115.7	C(20)	C(30)	H(15)	119.4
O(5)	C(31)	C(1)	106.9(5)	O(5)	C(31)	C(13)	109.2(4)
O(5)	C(31)	H(33)	110.6	C(1)	C(31)	C(13)	108.6(4)
C(1)	C(31)	H(33)	109.5	C(13)	C(31)	H(33)	111.9
C(19)	C(32)	C(22)	119.0(7)	C(19)	C(32)	H(16)	118.6
C(22)	C(32)	H(16)	122.5				

Table 5. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle
C(6)	O(1)	C(25)	C(23)	17.7(5)
C(25)	O(1)	C(6)	C(9)	-39.7(4)
C(12)	N(1)	C(7)	C(9)	59.9(5)
O(2)	C(1)	C(31)	O(5)	17.1(6)
O(4)	C(1)	C(31)	O(5)	-166.7(4)
O(1)	C(6)	C(8)	C(15)	-157.3(5)
O(1)	C(6)	C(9)	C(7)	-73.0(4)
O(1)	C(6)	C(11)	C(17)	179.9(3)
C(8)	C(6)	C(9)	C(7)	168.5(4)
C(9)	C(6)	C(8)	C(15)	-43.0(7)
C(8)	C(6)	C(11)	C(17)	-60.8(7)
C(11)	C(6)	C(8)	C(15)	85.1(6)
C(9)	C(6)	C(11)	C(17)	66.6(6)
C(11)	C(6)	C(9)	C(7)	42.7(5)
N(1)	C(7)	C(9)	C(6)	170.4(4)
C(6)	C(8)	C(15)	C(21)	-178.2(5)
C(15)	C(8)	C(24)	C(29)	2.2(8)
C(6)	C(9)	C(23)	C(25)	-33.4(4)
C(6)	C(11)	C(17)	C(26)	-178.0(5)
C(17)	C(11)	C(27)	C(28)	0.2(6)
C(20)	C(13)	C(22)	C(32)	-0.0(10)
C(20)	C(13)	C(31)	O(5)	166.3(5)
C(31)	C(13)	C(20)	C(30)	178.1(6)
C(22)	C(13)	C(31)	C(1)	98.0(7)
C(8)	C(15)	C(21)	C(16)	-0.2(6)
C(29)	C(16)	C(21)	C(15)	-0.1(7)
C(26)	C(18)	C(28)	C(27)	-1.1(11)
C(30)	C(19)	C(32)	C(22)	6.7(12)
C(13)	C(20)	C(30)	C(19)	-0.4(11)
C(9)	C(23)	C(25)	O(1)	11.4(4)
C(11)	C(27)	C(28)	C(18)	-0.1(8)

atom1	atom2	atom3	atom4	angle
C(25)	O(1)	C(6)	C(8)	80.7(5)
C(25)	O(1)	C(6)	C(11)	-160.3(4)
C(14)	N(1)	C(7)	C(9)	179.5(4)
O(2)	C(1)	C(31)	C(13)	-100.6(6)
O(4)	C(1)	C(31)	C(13)	75.7(6)
O(1)	C(6)	C(8)	C(24)	25.3(7)
O(1)	C(6)	C(9)	C(23)	45.1(4)
O(1)	C(6)	C(11)	C(27)	1.0(7)
C(8)	C(6)	C(9)	C(23)	-73.4(5)
C(9)	C(6)	C(8)	C(24)	139.6(5)
C(8)	C(6)	C(11)	C(27)	120.3(5)
C(11)	C(6)	C(8)	C(24)	-92.2(6)
C(9)	C(6)	C(11)	C(27)	-112.3(6)
C(11)	C(6)	C(9)	C(23)	160.8(4)
N(1)	C(7)	C(9)	C(23)	60.3(5)
C(6)	C(8)	C(24)	C(29)	180(179)
C(24)	C(8)	C(15)	C(21)	-0.8(8)
C(7)	C(9)	C(23)	C(25)	83.4(5)
C(6)	C(11)	C(27)	C(28)	179.1(5)
C(27)	C(11)	C(17)	C(26)	0.9(8)
C(22)	C(13)	C(20)	C(30)	2.6(10)
C(20)	C(13)	C(31)	C(1)	-77.5(7)
C(22)	C(13)	C(31)	O(5)	-18.2(8)
C(31)	C(13)	C(22)	C(32)	-175.3(6)
C(21)	C(16)	C(29)	C(24)	1.4(9)
C(11)	C(17)	C(26)	C(18)	-2.2(9)
C(28)	C(18)	C(26)	C(17)	2.3(11)
C(32)	C(19)	C(30)	C(20)	-4.3(13)
C(13)	C(22)	C(32)	C(19)	-4.8(11)
C(8)	C(24)	C(29)	C(16)	-2.5(9)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 6. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
O(1)	H(2)[1)]	3.297	O(1)	H(17)[1)]	3.190
O(1)	H(27)[1)]	3.011	O(1)	H(29)[1)]	3.352
O(2)	N(1)	2.645(6)	O(2)	C(12)	3.389(6)
O(2)	C(14)	3.308(6)	O(2)	C(16)[2)]	3.434(8)
O(2)	C(20)[3)]	3.420(8)	O(2)	C(23)	3.379(6)
O(2)	C(29)[2)]	3.400(7)	O(2)	H(1)	1.47(6)
O(2)	H(3)[2)]	2.805	O(2)	H(7)[3)]	2.552
O(2)	H(14)[2)]	2.775	O(2)	H(15)[3)]	3.565
O(2)	H(21)	2.458	O(2)	H(27)	3.225
O(2)	H(28)	3.577	O(2)	H(31)	2.987
O(4)	N(1)	3.181(6)	O(4)	C(7)	3.512(6)
O(4)	C(12)[1)]	3.235(7)	O(4)	C(14)	3.299(6)
O(4)	C(16)[4)]	3.550(7)	O(4)	H(1)	2.59(5)
O(4)	H(3)[4)]	2.796	O(4)	H(8)[4)]	3.231
O(4)	H(14)[2)]	3.245	O(4)	H(18)	2.956
O(4)	H(21)	3.199	O(4)	H(22)	2.870
O(4)	H(27)[1)]	2.809	O(4)	H(28)[1)]	2.784
O(4)	H(31)	3.140	O(4)	H(32)	3.060
O(5)	C(12)[5)]	3.533(6)	O(5)	C(28)[6)]	3.494(7)
O(5)	H(7)[3)]	3.255	O(5)	H(13)[6)]	3.101
O(5)	H(14)[2)]	3.483	O(5)	H(28)[5)]	3.424
O(5)	H(29)[5)]	2.889	O(5)	H(30)[5)]	2.882
N(1)	O(2)	2.645(6)	N(1)	O(4)	3.181(6)
N(1)	C(1)	3.256(8)	C(1)	N(1)	3.256(8)
C(1)	H(1)	2.28(6)	C(1)	H(3)[4)]	3.567
C(1)	H(14)[2)]	2.823	C(1)	H(18)	3.594
C(1)	H(21)	2.861	C(1)	H(22)	3.163
C(1)	H(31)	3.337	C(7)	O(4)	3.512(6)
C(9)	H(12)[3)]	3.475	C(11)	H(6)[7)]	3.225
C(12)	O(2)	3.389(6)	C(12)	O(4)[3)]	3.235(7)
C(12)	O(5)[8)]	3.533(6)	C(12)	H(3)[2)]	3.577
C(12)	H(12)[3)]	3.215	C(12)	H(18)[3)]	3.143
C(12)	H(22)[3)]	3.438	C(13)	H(22)	3.141
C(13)	H(30)[6)]	3.597	C(13)	H(32)[6)]	3.098
C(14)	O(2)	3.308(6)	C(14)	O(4)	3.299(6)
C(14)	C(30)[9)]	3.554(10)	C(14)	H(9)[8)]	3.229
C(15)	H(5)[10)]	3.226	C(15)	H(10)[3)]	3.185

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(15)	H(16)$^{11)}$	2.980	C(16)	O(2)$^{12)}$	3.434(8)
C(16)	O(4)$^{13)}$	3.550(7)	C(16)	H(5)$^{10)}$	3.420
C(16)	H(26)$^{12)}$	3.599	C(16)	H(28)$^{12)}$	3.567
C(16)	H(31)$^{12)}$	3.014	C(17)	H(6)$^{7)}$	3.261
C(17)	H(13)$^{3)}$	3.294	C(17)	H(16)$^{11)}$	3.351
C(18)	H(6)$^{7)}$	3.236	C(18)	H(33)$^{9)}$	3.415
C(19)	H(23)	3.399	C(19)	H(30)$^{6)}$	3.527
C(19)	H(31)$^{6)}$	3.485	C(19)	H(32)$^{6)}$	3.449
C(20)	O(2)$^{1)}$	3.420(8)	C(20)	H(22)	2.872
C(20)	H(26)$^{1)}$	3.470	C(20)	H(30)$^{6)}$	3.138
C(20)	H(32)$^{6)}$	3.266	C(21)	H(5)$^{10)}$	2.915
C(21)	H(10)$^{3)}$	3.140	C(21)	H(14)$^{3)}$	3.512
C(21)	H(16)$^{11)}$	2.995	C(22)	H(15)$^{3)}$	3.150
C(22)	H(22)	3.569	C(22)	H(28)$^{5)}$	3.452
C(22)	H(30)$^{5)}$	3.311	C(22)	H(32)$^{6)}$	3.155
C(23)	O(2)	3.379(6)	C(23)	H(11)$^{10)}$	3.530
C(23)	H(15)$^{3)}$	3.271	C(24)	H(2)$^{1)}$	3.534
C(24)	H(5)$^{14)}$	3.445	C(24)	H(8)$^{1)}$	3.141
C(24)	H(11)$^{10)}$	3.509	C(25)	H(27)$^{1)}$	3.177
C(26)	H(6)$^{7)}$	3.284	C(26)	H(13)$^{3)}$	3.319
C(26)	H(20)$^{11)}$	3.350	C(27)	H(2)$^{1)}$	3.494
C(27)	H(4)$^{1)}$	3.335	C(27)	H(6)$^{7)}$	3.169
C(27)	H(17)$^{1)}$	3.547	C(27)	H(29)$^{1)}$	3.109
C(28)	O(5)$^{9)}$	3.494(7)	C(28)	H(4)$^{1)}$	3.301
C(28)	H(6)$^{7)}$	3.183	C(28)	H(26)$^{9)}$	3.538
C(28)	H(33)$^{9)}$	3.293	C(29)	O(2)$^{12)}$	3.400(7)
C(29)	H(8)$^{1)}$	3.173	C(29)	H(11)$^{10)}$	3.504
C(29)	H(13)$^{14)}$	3.576	C(29)	H(26)$^{12)}$	3.393
C(29)	H(31)$^{12)}$	2.939	C(30)	C(14)$^{6)}$	3.554(10)
C(30)	H(9)$^{1)}$	3.187	C(30)	H(21)$^{1)}$	3.511
C(30)	H(22)	3.120	C(30)	H(23)	3.431
C(30)	H(30)$^{6)}$	3.081	C(30)	H(32)$^{6)}$	3.398
C(31)	H(14)$^{2)}$	3.461	C(32)	H(4)$^{10)}$	3.556
C(32)	H(8)$^{10)}$	3.409	C(32)	H(23)	3.552
C(32)	H(32)$^{6)}$	3.382	H(1)	O(2)	1.47(6)
H(1)	O(4)	2.59(5)	H(1)	C(1)	2.28(6)
H(1)	H(3)$^{2)}$	3.002	H(1)	H(7)$^{3)}$	3.120

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(1)	H(14)[2]	3.423	H(1)	H(26)	3.571
H(2)	O(1)[3]	3.297	H(2)	C(24)[3]	3.534
H(2)	C(27)[3]	3.494	H(2)	H(5)[10]	3.405
H(2)	H(10)[3]	2.673	H(2)	H(12)[3]	2.886
H(2)	H(16)[11]	2.927	H(3)	O(2)[12]	2.805
H(3)	O(4)[13]	2.796	H(3)	C(1)[13]	3.567
H(3)	C(12)[12]	3.577	H(3)	H(1)[12]	3.002
H(3)	H(7)[13]	3.148	H(3)	H(26)[12]	3.163
H(3)	H(28)[12]	3.012	H(3)	H(31)[12]	2.943
H(3)	H(33)[13]	3.084	H(4)	C(27)[3]	3.335
H(4)	C(28)[3]	3.301	H(4)	C(32)[11]	3.556
H(4)	H(12)[3]	2.885	H(4)	H(13)[3]	2.846
H(4)	H(16)[11]	2.748	H(5)	C(15)[11]	3.226
H(5)	C(16)[11]	3.420	H(5)	C(21)[11]	2.915
H(5)	C(24)[7]	3.445	H(5)	H(2)[11]	3.405
H(5)	H(8)[11]	2.927	H(5)	H(10)[7]	2.801
H(5)	H(14)[7]	3.202	H(5)	H(20)[11]	3.342
H(5)	H(23)[7]	3.332	H(5)	H(33)[9]	3.514
H(6)	C(11)[14]	3.225	H(6)	C(17)[14]	3.261
H(6)	C(18)[14]	3.236	H(6)	C(26)[14]	3.284
H(6)	C(27)[14]	3.169	H(6)	C(28)[14]	3.183
H(7)	O(2)[1]	2.552	H(7)	O(5)[1]	3.255
H(7)	H(1)[1]	3.120	H(7)	H(3)[4]	3.148
H(7)	H(21)[1]	3.342	H(7)	H(22)	3.115
H(7)	H(26)[1]	2.771	H(7)	H(27)[1]	3.182
H(7)	H(30)[6]	3.358	H(8)	O(4)[13]	3.231
H(8)	C(24)[3]	3.141	H(8)	C(29)[3]	3.173
H(8)	C(32)[11]	3.409	H(8)	H(5)[10]	2.927
H(8)	H(10)[3]	2.606	H(8)	H(14)[3]	2.661
H(8)	H(16)[11]	2.932	H(8)	H(31)[13]	3.591
H(9)	C(14)[5]	3.229	H(9)	C(30)[3]	3.187
H(9)	H(15)[3]	2.631	H(9)	H(28)[5]	2.936
H(9)	H(29)[5]	3.559	H(9)	H(30)[5]	2.386
H(9)	H(31)[5]	3.320	H(9)	H(32)[6]	3.550
H(10)	C(15)[1]	3.185	H(10)	C(21)[1]	3.140
H(10)	H(2)[1]	2.673	H(10)	H(5)[14]	2.801
H(10)	H(8)[1]	2.606	H(11)	C(23)[11]	3.530

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(11)	C(24)[11]	3.509	H(11)	C(29)[11]	3.504
H(11)	H(13)[3]	2.874	H(11)	H(20)[11]	2.719
H(11)	H(23)[11]	3.021	H(12)	C(9)[1]	3.475
H(12)	C(12)[1]	3.215	H(12)	H(2)[1]	2.886
H(12)	H(4)[1]	2.885	H(12)	H(17)[1]	2.612
H(12)	H(19)[1]	3.504	H(12)	H(27)[1]	3.218
H(12)	H(29)[1]	2.417	H(13)	O(5)[9]	3.101
H(13)	C(17)[1]	3.294	H(13)	C(26)[1]	3.319
H(13)	C(29)[7]	3.576	H(13)	H(4)[1]	2.846
H(13)	H(11)[1]	2.874	H(13)	H(14)[7]	3.209
H(13)	H(26)[9]	2.929	H(13)	H(33)[9]	3.322
H(14)	O(2)[12]	2.775	H(14)	O(4)[12]	3.245
H(14)	O(5)[12]	3.483	H(14)	C(1)[12]	2.823
H(14)	C(21)[1]	3.512	H(14)	C(31)[12]	3.461
H(14)	H(1)[12]	3.423	H(14)	H(5)[14]	3.202
H(14)	H(8)[1]	2.661	H(14)	H(13)[14]	3.209
H(14)	H(26)[12]	2.788	H(14)	H(31)[12]	2.832
H(14)	H(33)[12]	3.408	H(15)	O(2)[1]	3.565
H(15)	C(22)[1]	3.150	H(15)	C(23)[1]	3.271
H(15)	H(9)[1]	2.631	H(15)	H(16)[1]	3.509
H(15)	H(20)[1]	2.876	H(15)	H(21)[1]	2.802
H(15)	H(22)	3.503	H(15)	H(30)[6]	3.248
H(16)	C(15)[10]	2.980	H(16)	C(17)[10]	3.351
H(16)	C(21)[10]	2.995	H(16)	H(2)[10]	2.927
H(16)	H(4)[10]	2.748	H(16)	H(8)[10]	2.932
H(16)	H(15)[3]	3.509	H(17)	O(1)[3]	3.190
H(17)	C(27)[3]	3.547	H(17)	H(12)[3]	2.612
H(18)	O(4)	2.956	H(18)	C(1)	3.594
H(18)	C(12)[1]	3.143	H(18)	H(27)[1]	2.903
H(18)	H(28)[1]	3.044	H(18)	H(29)[1]	2.952
H(19)	H(12)[3]	3.504	H(19)	H(26)[8]	3.558
H(20)	C(26)[10]	3.350	H(20)	H(5)[10]	3.342
H(20)	H(11)[10]	2.719	H(20)	H(15)[3]	2.876
H(21)	O(2)	2.458	H(21)	O(4)	3.199
H(21)	C(1)	2.861	H(21)	C(30)[3]	3.511
H(21)	H(7)[3]	3.342	H(21)	H(15)[3]	2.802
H(22)	O(4)	2.870	H(22)	C(1)	3.163

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(22)	C(12)[1)]	3.438	H(22)	C(13)	3.141
H(22)	C(20)	2.872	H(22)	C(22)	3.569
H(22)	C(30)	3.120	H(22)	H(7)	3.115
H(22)	H(15)	3.503	H(22)	H(27)[1)]	2.545
H(23)	C(19)	3.399	H(23)	C(30)	3.431
H(23)	C(32)	3.552	H(23)	H(5)[14)]	3.332
H(23)	H(11)[10)]	3.021	H(26)	C(16)[2)]	3.599
H(26)	C(20)[3)]	3.470	H(26)	C(28)[6)]	3.538
H(26)	C(29)[2)]	3.393	H(26)	H(1)	3.571
H(26)	H(3)[2)]	3.163	H(26)	H(7)[3)]	2.771
H(26)	H(13)[6)]	2.929	H(26)	H(14)[2)]	2.788
H(26)	H(19)[5)]	3.558	H(26)	H(29)[5)]	3.443
H(26)	H(30)[5)]	3.224	H(27)	O(1)[3)]	3.011
H(27)	O(2)	3.225	H(27)	O(4)[3)]	2.809
H(27)	C(25)[3)]	3.177	H(27)	H(7)[3)]	3.182
H(27)	H(12)[3)]	3.218	H(27)	H(18)[3)]	2.903
H(27)	H(22)[3)]	2.545	H(28)	O(2)	3.577
H(28)	O(4)[3)]	2.784	H(28)	O(5)[8)]	3.424
H(28)	C(16)[2)]	3.567	H(28)	C(22)[8)]	3.452
H(28)	H(3)[2)]	3.012	H(28)	H(9)[8)]	2.936
H(28)	H(18)[3)]	3.044	H(28)	H(32)[3)]	3.163
H(29)	O(1)[3)]	3.352	H(29)	O(5)[8)]	2.889
H(29)	C(27)[3)]	3.109	H(29)	H(9)[8)]	3.559
H(29)	H(12)[3)]	2.417	H(29)	H(18)[3)]	2.952
H(29)	H(26)[8)]	3.443	H(30)	O(5)[8)]	2.882
H(30)	C(13)[9)]	3.597	H(30)	C(19)[9)]	3.527
H(30)	C(20)[9)]	3.138	H(30)	C(22)[8)]	3.311
H(30)	C(30)[9)]	3.081	H(30)	H(7)[9)]	3.358
H(30)	H(9)[8)]	2.386	H(30)	H(15)[9)]	3.248
H(30)	H(26)[8)]	3.224	H(31)	O(2)	2.987
H(31)	O(4)	3.140	H(31)	C(1)	3.337
H(31)	C(16)[2)]	3.014	H(31)	C(19)[9)]	3.485
H(31)	C(29)[2)]	2.939	H(31)	H(3)[2)]	2.943
H(31)	H(8)[4)]	3.591	H(31)	H(9)[8)]	3.320
H(31)	H(14)[2)]	2.832	H(32)	O(4)	3.060
H(32)	C(13)[9)]	3.098	H(32)	C(19)[9)]	3.449
H(32)	C(20)[9)]	3.266	H(32)	C(22)[9)]	3.155

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(32)	C(30)[9]	3.398	H(32)	C(32)[9]	3.382
H(32)	H(9)[9]	3.550	H(32)	H(28)[1]	3.163
H(33)	C(18)[6]	3.415	H(33)	C(28)[6]	3.293
H(33)	H(3)[4]	3.084	H(33)	H(5)[6]	3.514
H(33)	H(13)[6]	3.322	H(33)	H(14)[2]	3.408

Symmetry Operators:

(1) X+1,Y,Z
(2) X,Y,Z+1
(3) X-1,Y,Z
(4) X+1,Y,Z+1
(5) -X+1,Y+1/2,-Z+1
(6) -X+2,Y+1/2,-Z+1
(7) -X+2,Y+1/2-1,-Z
(8) -X+1,Y+1/2-1,-Z+1
(9) -X+2,Y+1/2-1,-Z+1
(10) -X+1,Y+1/2,-Z
(11) -X+1,Y+1/2-1,-Z
(12) X,Y,Z-1
(13) X-1,Y,Z-1
(14) -X+2,Y+1/2,-Z

Intramolecular and Intermolecular Hydrogen bonds

D	H	A	D...A	D-H	H...A	D-H...A
O(5)	H(26)	O(2)	2.581(5)	0.950	2.148	106.2
N(1)	H(1)	O(2)	2.645(6)	1.19(7)	1.47(6)	167(4)
N(1)	H(1)	O(4)	3.181(6)	1.19(7)	2.59(5)	109(3)

Note) 1. The symmetry operations are applied to the acceptors.
2. Estimated standard deviations (esd's) are shown in the parentheses.
They are not calculated when all atoms have an esd=0.0.

Absolute configuration analysis

	H	K	L	Fo diff	Fc diff	Fc diff/sigma
Incorrect:	0	-2	2	0.16	-0.12	-0.24
Correct trend:	1	-8	1	-0.11	-0.10	-0.20
Correct trend:	0	-2	2	-0.15	-0.12	-0.20
Correct trend:	0	-2	2	-0.07	-0.12	-0.20
Incorrect:	0	-2	2	0.37	-0.12	-0.17
Incorrect:	1	-8	1	0.64	-0.10	-0.17
Correct trend:	2	-1	1	-0.40	-0.05	-0.17
Correct trend:	0	-2	2	-0.97	-0.12	-0.17

Incorrect:	0	-2	2	0.21	-0.12	-0.16
Correct trend:	0	-2	2	-0.59	-0.12	-0.15
Correct trend:	1	-8	1	-0.96	-0.10	-0.15
Correct trend:	2	-2	2	-1.42	-0.12	-0.13
Incorrect:	-1	-2	3	-0.17	0.15	0.13
Incorrect:	-2	-4	2	-0.48	0.10	0.13
Correct trend:	-3	-5	2	-0.46	-0.08	-0.13
Incorrect:	0	-2	2	1.57	-0.12	-0.13
Correct trend:	-3	-5	2	-1.21	-0.08	-0.12
Correct trend:	-3	-2	2	-1.50	-0.08	-0.12
Correct trend:	-1	-2	3	1.64	0.15	0.12
Correct trend:	2	-2	2	-0.27	-0.12	-0.12
Incorrect:	-1	-3	5	0.84	-0.10	-0.12
Correct trend:	1	-7	1	-0.02	-0.07	-0.12
Correct trend:	-1	-2	3	4.31	0.15	0.12
Correct trend:	-1	-2	3	0.52	0.15	0.12
Incorrect:	2	-2	2	1.97	-0.12	-0.11
Incorrect:	1	-3	3	1.18	-0.07	-0.11
Correct trend:	-2	-4	2	1.29	0.10	0.11
Correct trend:	0	-5	2	-0.14	-0.10	-0.11
Incorrect:	-3	-2	2	0.42	-0.08	-0.11
Correct trend:	2	-2	2	-0.06	-0.12	-0.11
Incorrect:	-1	-2	3	-0.19	0.15	0.11
Incorrect:	1	-4	2	-2.43	0.13	0.11
Correct trend:	0	-5	2	-3.14	-0.10	-0.11
Correct trend:	-1	-2	3	1.32	0.15	0.11
Correct trend:	-1	-2	3	0.33	0.15	0.11
Incorrect:	-1	-2	3	-1.47	0.15	0.11
Incorrect:	1	-4	2	-3.34	0.13	0.11
Correct trend:	1	-10	1	0.41	0.10	0.11
Correct trend:	-3	-2	2	-0.70	-0.08	-0.11
Incorrect:	1	-10	1	-0.23	0.10	0.11
Correct trend:	1	-4	2	0.67	0.13	0.11
Incorrect:	-1	-2	3	-1.92	0.15	0.11
Incorrect:	-2	-4	2	-0.93	0.10	0.10
Incorrect:	-2	-4	2	-0.08	0.10	0.10
Incorrect:	0	-5	2	0.83	-0.10	-0.10
Incorrect:	-1	-3	5	1.21	-0.10	-0.10
Incorrect:	1	-3	3	0.71	-0.07	-0.10
Correct trend:	0	-5	2	-1.18	-0.10	-0.10
Correct trend:	1	-4	2	1.38	0.13	0.10
Incorrect:	1	-7	1	0.29	-0.07	-0.10
Correct trend:	-1	-8	1	-0.82	-0.10	-0.10
Correct trend:	1	-7	1	-0.66	-0.07	-0.10
Correct trend:	0	-5	2	-1.09	-0.10	-0.10
Correct trend:	1	-7	1	-0.57	-0.07	-0.10
Correct trend:	-1	-8	1	-2.23	-0.10	-0.10
Incorrect:	-1	-3	5	0.46	-0.10	-0.10
Correct trend:	-3	-2	2	-0.41	-0.08	-0.10
Incorrect:	2	-5	0	0.54	-0.07	-0.10
Incorrect:	-1	-3	5	0.47	-0.10	-0.10
Correct trend:	1	-4	2	1.19	0.13	0.10
Incorrect:	2	-2	2	0.78	-0.12	-0.10
Incorrect:	1	-4	2	-0.39	0.13	0.10
Correct trend:	-2	-1	1	0.48	0.09	0.10
Incorrect:	2	-4	1	0.60	-0.07	-0.10

Correct trend:	2	-2	2	-0.13	-0.12	-0.10
Incorrect:	1	-3	3	0.43	-0.07	-0.10
Incorrect:	-1	-7	2	0.50	-0.09	-0.09
Correct trend:	2	-2	2	-0.52	-0.12	-0.09
Correct trend:	-3	-2	2	-0.38	-0.08	-0.09
Incorrect:	3	-2	1	0.24	-0.08	-0.09
Correct trend:	-2	-1	1	0.11	0.09	0.09
Incorrect:	-1	-6	1	-1.39	0.08	0.09
Correct trend:	2	-4	1	-1.17	-0.07	-0.09
Incorrect:	-1	-3	5	1.04	-0.10	-0.09
Incorrect:	-1	-7	2	2.91	-0.09	-0.09
Incorrect:	1	-4	2	-0.55	0.13	0.09
Correct trend:	2	-3	0	-0.77	-0.07	-0.09
Incorrect:	0	-5	2	0.12	-0.10	-0.09
Correct trend:	2	-4	1	-0.26	-0.07	-0.09
Incorrect:	-1	-6	1	-0.65	0.08	0.09
Correct trend:	-1	-6	1	0.36	0.08	0.09
Incorrect:	2	-5	0	0.14	-0.07	-0.09
Correct trend:	1	-4	2	0.01	0.13	0.09
Incorrect:	-3	-5	4	0.43	-0.06	-0.09
Correct trend:	-2	-4	2	1.20	0.10	0.09
Correct trend:	1	-5	2	4.85	0.08	0.09
Correct trend:	-2	-1	1	0.27	0.09	0.09
Correct trend:	-1	-8	1	-0.89	-0.10	-0.09
Incorrect:	-1	-8	1	1.52	-0.10	-0.09
Correct trend:	2	-3	0	-0.21	-0.07	-0.09
Incorrect:	-1	-3	5	0.01	-0.10	-0.09
Correct trend:	0	-1	4	-1.15	-0.07	-0.09
Correct trend:	-1	-3	5	-0.21	-0.10	-0.09
Correct trend:	-2	-4	2	0.20	0.10	0.09
Incorrect:	2	-5	0	0.67	-0.07	-0.09
Incorrect:	-2	-4	2	-1.47	0.10	0.09
Incorrect:	2	-4	1	0.07	-0.07	-0.09
Incorrect:	-1	-7	2	0.23	-0.09	-0.08
Correct trend:	-2	-1	1	0.65	0.09	0.08
Incorrect:	2	-3	0	0.38	-0.07	-0.08
Incorrect:	2	-4	1	1.92	-0.07	-0.08
Incorrect:	3	-2	1	0.09	-0.08	-0.08
Correct trend:	-1	-6	1	2.87	0.08	0.08
Incorrect:	2	-9	1	1.22	-0.07	-0.08
Correct trend:	-2	-1	1	0.60	0.09	0.08
Correct trend:	-1	-3	5	-1.80	-0.10	-0.08
Correct trend:	2	-4	1	-0.06	-0.07	-0.08
Correct trend:	2	-3	0	-0.10	-0.07	-0.08
Incorrect:	1	-10	1	-0.20	0.10	0.08
Incorrect:	3	-2	1	0.52	-0.08	-0.08
Incorrect:	3	-2	1	0.03	-0.08	-0.08
Incorrect:	0	-8	1	-4.65	0.08	0.08
Incorrect:	-1	-5	4	2.17	-0.08	-0.08
Correct trend:	2	-9	1	-0.91	-0.07	-0.08
Correct trend:	1	-3	3	-2.16	-0.07	-0.08
Incorrect:	1	-7	2	1.02	-0.07	-0.08
Correct trend:	-1	-6	1	2.10	0.08	0.08
Incorrect:	-1	-8	1	0.49	-0.10	-0.08
Incorrect:	3	-2	1	0.43	-0.08	-0.08
Correct trend:	-2	-1	1	0.22	0.09	0.08

Correct trend:	-1	-7	2	-0.95	-0.09	-0.08
Incorrect:	2	-4	1	0.79	-0.07	-0.07
Correct trend:	3	-2	1	-0.50	-0.08	-0.07
Correct trend:	1	-10	1	0.59	0.10	0.07
Incorrect:	-2	-1	1	0.00	0.09	0.07
Correct trend:	2	-3	0	-0.74	-0.07	-0.07
Incorrect:	-1	-6	3	-0.03	0.04	0.07
Correct trend:	-1	-5	1	-0.09	-0.10	-0.07
Incorrect:	2	-3	0	0.69	-0.07	-0.07
Incorrect:	1	-6	4	1.02	-0.11	-0.07
Incorrect:	-2	-4	3	-0.29	0.05	0.07
Incorrect:	-2	-1	1	-0.75	0.09	0.07
Correct trend:	2	-5	0	-0.37	-0.07	-0.07
Correct trend:	3	-2	1	-0.16	-0.08	-0.07
Correct trend:	-1	-8	1	-0.76	-0.10	-0.07
Correct trend:	2	-5	0	-0.06	-0.07	-0.07
Incorrect:	2	-3	0	0.04	-0.07	-0.07
Incorrect:	3	-2	1	0.11	-0.08	-0.07
Incorrect:	-1	-7	2	0.44	-0.09	-0.07
Correct trend:	1	-6	5	0.01	0.05	0.07
Correct trend:	2	-5	0	-0.57	-0.07	-0.07
Correct trend:	1	-3	3	-0.66	-0.07	-0.07
Incorrect:	-1	-3	5	0.30	-0.10	-0.07
Incorrect:	-2	-1	1	-4.49	0.09	0.07
Incorrect:	-2	-6	2	0.00	-0.06	-0.07
Correct trend:	2	-4	1	-0.31	-0.07	-0.07
Incorrect:	1	-3	3	4.46	-0.07	-0.07
Correct trend:	1	-5	2	5.63	0.08	0.07
Correct trend:	0	-10	1	0.10	0.07	0.07
Correct trend:	1	-3	3	-0.23	-0.07	-0.07
Correct trend:	-2	-6	2	-0.78	-0.06	-0.07
Correct trend:	2	-3	0	-0.68	-0.07	-0.07
Incorrect:	-1	-7	2	0.72	-0.09	-0.07
Correct trend:	0	-8	1	0.14	0.08	0.07
Incorrect:	-2	-1	2	0.18	-0.04	-0.07
Incorrect:	1	-4	1	-0.46	0.07	0.07
Correct trend:	-2	-1	2	-0.06	-0.04	-0.07
Correct trend:	-1	-3	4	0.55	0.06	0.07
Incorrect:	-1	-5	1	0.82	-0.10	-0.07
Incorrect:	1	-6	4	0.40	-0.11	-0.07
Incorrect:	1	-5	2	-0.05	0.08	0.07
Correct trend:	0	-1	4	-1.02	-0.07	-0.07
Incorrect:	-1	-7	2	1.44	-0.09	-0.07
Correct trend:	-2	-6	2	-0.33	-0.06	-0.07
Correct trend:	3	-4	1	-0.29	-0.10	-0.07
Correct trend:	0	-1	4	-0.26	-0.07	-0.07
Correct trend:	1	-8	0	0.05	0.03	0.07
Correct trend:	1	-7	2	-0.12	-0.07	-0.07
Incorrect:	-3	-5	4	1.36	-0.06	-0.07
Correct trend:	1	-4	0	-1.06	-0.07	-0.07
Correct trend:	0	-1	4	-0.11	-0.07	-0.07
Correct trend:	0	-3	3	-2.95	-0.04	-0.07
Incorrect:	0	-8	1	-0.56	0.08	0.07
Correct trend:	1	-4	0	-0.67	-0.07	-0.07
Incorrect:	1	-3	3	0.42	-0.07	-0.07
Incorrect:	0	-1	4	0.58	-0.07	-0.07

Incorrect:	1	-12	3	3.11	-0.08	-0.07
Correct trend:	3	-4	1	-0.79	-0.10	-0.06
Incorrect:	3	-3	1	0.65	-0.08	-0.06
Correct trend:	0	-1	4	-0.68	-0.07	-0.06
Correct trend:	0	-8	1	0.96	0.08	0.06
Correct trend:	-2	-1	2	-0.10	-0.04	-0.06
Correct trend:	-1	-5	1	-0.34	-0.10	-0.06
Correct trend:	1	-4	0	-0.25	-0.07	-0.06
Incorrect:	1	-5	2	-0.24	0.08	0.06
Incorrect:	-1	-5	1	0.93	-0.10	-0.06
Incorrect:	1	-4	0	0.44	-0.07	-0.06
Correct trend:	1	-4	0	-1.32	-0.07	-0.06
Correct trend:	-1	-8	5	-0.06	-0.09	-0.06
Correct trend:	1	-5	2	3.21	0.08	0.06
Correct trend:	-2	-1	2	-0.34	-0.04	-0.06
Correct trend:	1	-10	3	0.71	0.07	0.06
Correct trend:	-1	-10	4	-0.08	-0.06	-0.06
Correct trend:	2	-7	0	1.32	0.06	0.06
Correct trend:	1	-7	2	-0.37	-0.07	-0.06
Correct trend:	-1	-5	1	-1.37	-0.10	-0.06
Incorrect:	1	-4	0	0.18	-0.07	-0.06
Incorrect:	-1	-5	1	0.82	-0.10	-0.06
Incorrect:	-2	-1	2	0.43	-0.04	-0.06
Incorrect:	-3	-2	2	3.78	-0.08	-0.06

Summary	Total	Sum delta(Fc)	<average>
Number of reflections processed:	6669		
Fc difference agrees with Fo:	1084	40.790	0.038
Fc difference disagrees with Fo:	1002	37.650	0.038
F(H)=F(-H) reflexions:	348		
Reflections without Friedel mates:	1800		
Weak reflections:	0		

Significant Diff*:	<0.5	0.5-1.0	1.0-2.0	2.0-3.0	3.0-4.0	>4.0
Correct trend:	1084	0	0	0	0	0
Incorrect:	1002	0	0	0	0	0

* Significant Diff = ||Fc(+)|-|Fc(-)||/sqrt(sigma[Fo(+)]**2+sigma[Fo(-)]**2)