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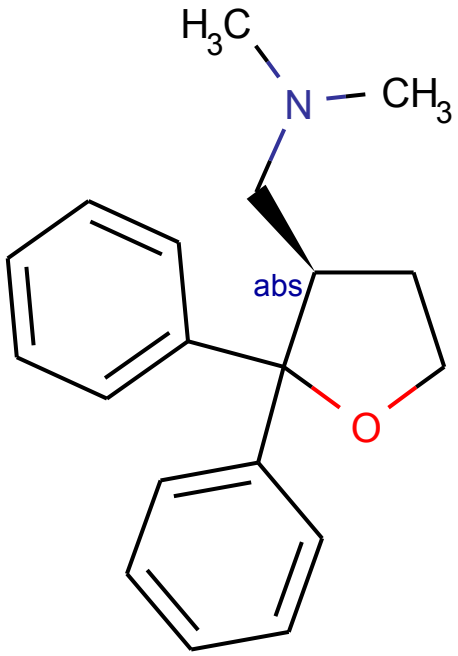
FLE0592_1

Submitted by: Szokol Zsuzsanna
Operator: Dancso Andras

X-ray Structure Report



March 21, 2022

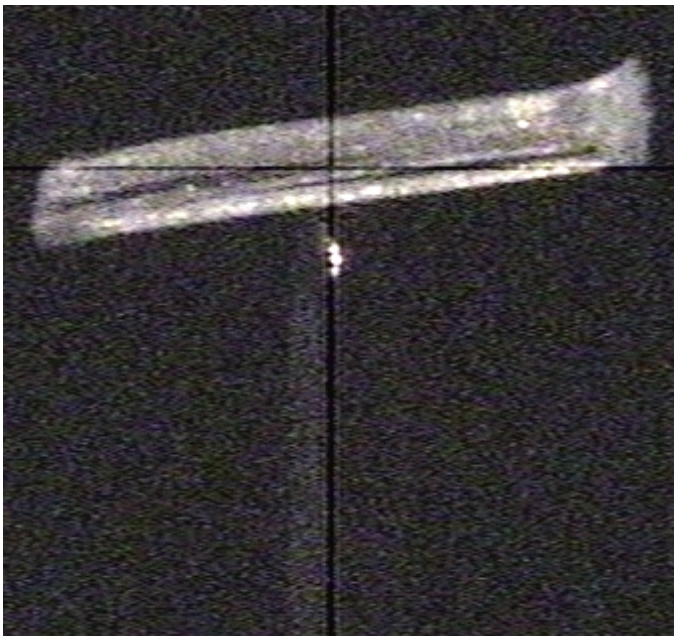


Fig. 1. The crystal

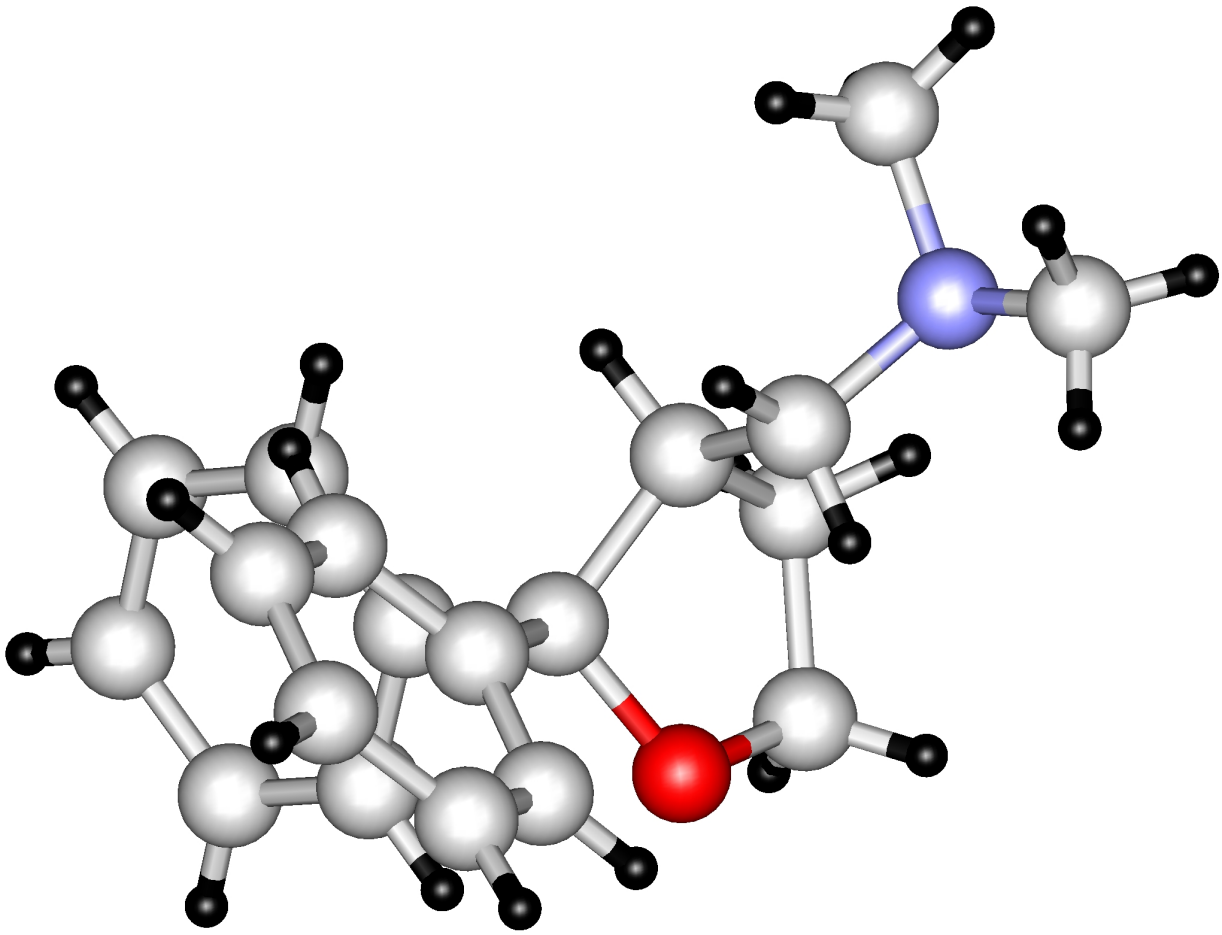


Fig. 2. The molecule (most hydrogens were generated by the software)

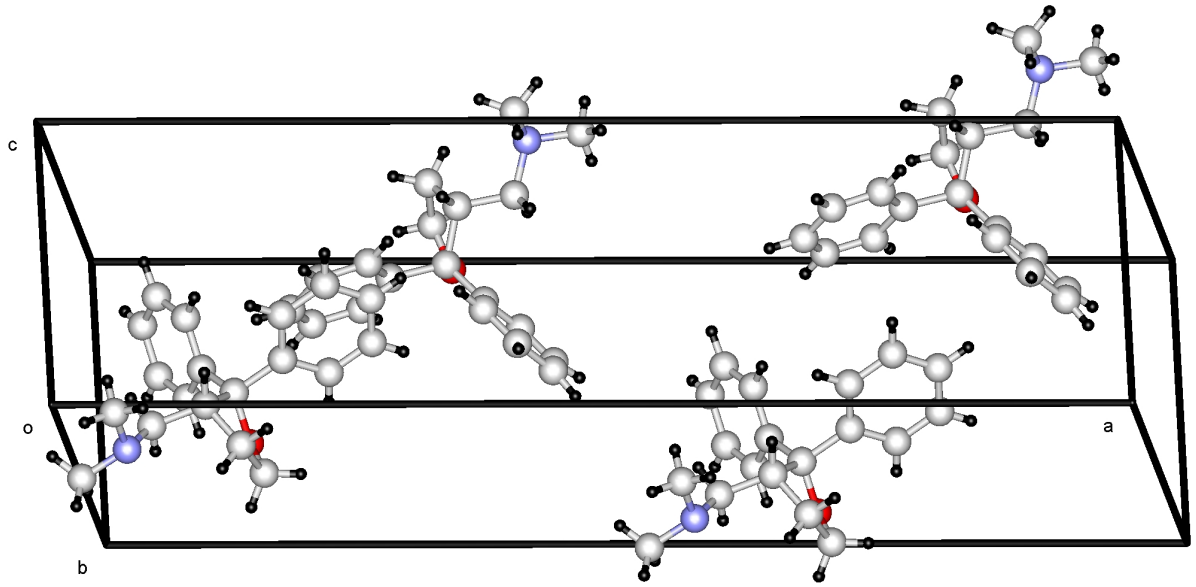


Fig. 3. Packing

Experimental

Data Collection

A colorless prism crystal of $C_{19}H_{23}NO$ having approximate dimensions of 0.93 x 0.17 x 0.16 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 C-centered monoclinic cell with dimensions:

a = 29.229(5) Å

b = 6.0958(10) Å β = 102.518(6)^o

c = 9.3517(15) Å

V = 1626.6(5) Å^3

For Z = 4 and F.W. = 281.40, the calculated density is 1.149 g/cm^3. Based on the systematic absences of:

hkl: h+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:

C2 (#5)

The data were collected at a temperature of 20 ± 1^{o}C to a maximum 2θ value of 143.0^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 12.0 [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 12.0 [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 12.0 [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 12.0 [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 12.0 [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 9344 reflections that were collected, 2829 were unique (R_{int} = 0.076).

The linear absorption coefficient, μ, for Cu-Kα radiation is 5.416 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.741 to 0.919. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F was based on 4829 observed reflections ($I > 2.00\sigma(I)$) and 217 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0570$$

$$R_W = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.0601$$

The standard deviation of an observation of unit weight[4] was 5.34. 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 1.66 and -1.78 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter -0.2(5).[5]

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10,11] crystallographic software package.

References

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

(2) 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.

(3) Least Squares function minimized:

$$\Sigma w(|F_O|-|F_C|)^2$$ where w = Least Squares weights.

(4) 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

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

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

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

(8) 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).

(9) 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).

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

(11) 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	$C_{19}H_{23}NO$
Formula Weight	281.40
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.93 X 0.17 X 0.16 mm
Crystal System	monoclinic
Lattice Type	C-centered
Indexing Images	4 oscillations @ 60.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 29.229(5) Å b = 6.0958(10) Å c = 9.3517(15) Å β = 102.518(6) ^{o} V = 1626.6(5) Å^{3}
Space Group	C2 (#5)
Z value	4
D_{calc}	1.149 g/cm^{3}
F_{000}	608.00
μ(CuKα)	5.416 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^{o}
Exposure Rate	12.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=0.0)	20.0 - 200.0^{o}
Exposure Rate	12.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=90.0)	20.0 - 200.0^{o}
Exposure Rate	12.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=180.0)	20.0 - 200.0^{o}
Exposure Rate	12.0 sec./^{o}
ω oscillation Range (χ=54.0, ϕ=270.0)	20.0 - 200.0^{o}
Exposure Rate	12.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	143.0^{o}
No. of Reflections Measured	Total: 9344 Unique: 2829 (R_{int} = 0.076) Friedel pairs: 1224
Corrections	Lorentz-polarization Absorption (trans. factors: 0.741 - 0.919)

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	143.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	4829
No. Variables	217
Reflection/Parameter Ratio	22.25
Residuals: R (I>2.00σ(I))	0.0570
Residuals: Rw (I>2.00σ(I))	0.0601
Goodness of Fit Indicator	5.342
Flack Parameter	-0.2(5)
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	1.66 e$^-$/Å^3
Minimum peak in Final Diff. Map	-1.78 e$^-$/Å^3

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

atom	x	y	z	B_{eq}
O(1)	0.33672(11)	0.9201(5)	0.9290(4)	4.89(11)
N(2)	0.43165(18)	0.4795(8)	1.1682(5)	5.65(16)
C(3)	0.2019(2)	0.5452(11)	0.6053(5)	4.82(19)
C(4)	0.37701(18)	0.6145(9)	0.6377(5)	4.65(16)
C(5)	0.2365(2)	0.3872(9)	0.6340(5)	5.18(19)
C(6)	0.3604(2)	0.5563(10)	0.9742(5)	4.18(17)
C(7)	0.37154(18)	0.7666(8)	0.7430(5)	3.82(15)
C(8)	0.29088(19)	0.6499(9)	0.7670(5)	3.26(15)
C(9)	0.2117(2)	0.7527(10)	0.6567(5)	5.3(2)
C(10)	0.4124(2)	0.5895(8)	1.0298(5)	5.16(17)
C(11)	0.2803(2)	0.4375(8)	0.7152(5)	4.68(18)
C(12)	0.2553(2)	0.8064(8)	0.7355(5)	4.67(17)
C(13)	0.3402(2)	0.7189(9)	0.8493(5)	3.96(16)
C(14)	0.39488(19)	0.9686(8)	0.7456(5)	4.79(18)
C(15)	0.3319(2)	0.6171(10)	1.0858(5)	6.5(2)
C(16)	0.4050(2)	0.6595(10)	0.5407(6)	5.6(2)
C(17)	0.4224(2)	1.0090(9)	0.6476(6)	5.9(2)
C(18)	0.4783(2)	0.5549(10)	1.2331(5)	7.9(2)
C(19)	0.3228(2)	0.8653(11)	1.0617(6)	7.0(2)
C(20)	0.4280(2)	0.8591(12)	0.5434(6)	6.0(2)
C(21)	0.4315(2)	0.2445(10)	1.1546(6)	11.1(2)
H(1)	0.4171	0.7428	1.0446	6.13
H(2)	0.4284	0.5409	0.9574	6.14
H(3)	0.3534(12)	0.408(6)	0.934(3)	3.1(12)
H(4)	0.1715	0.5082	0.5512	5.74
H(5)	0.3619	0.4761	0.6339	5.59
H(6)	0.2291	0.2450	0.5940	6.09
H(7)	0.1878	0.8608	0.6364	6.18
H(8)	0.3043	0.3298	0.7369	5.46
H(9)	0.2633	0.9512	0.7695	5.62
H(10)	0.3900	1.0725	0.8165	5.88
H(11)	0.4102	0.5565	0.4698	6.79
H(12)	0.4396	1.1426	0.6578	7.18
H(13)	0.4454	0.9004	0.4729	7.45
H(14)	0.3035	0.5354	1.0689	7.85
H(15)	0.3493	0.5895	1.1824	7.86
H(16)	0.3400	0.9474	1.1418	8.68

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

atom	x	y	z	B_{eq}
H(17)	0.2902	0.8935	1.0513	8.68
H(18)	0.5007	0.4702	1.1977	9.05
H(19)	0.4841	0.5442	1.3368	9.04
H(20)	0.4805	0.7040	1.2058	9.05
H(21)	0.4025	0.1874	1.1681	12.14
H(22)	0.4565	0.1787	1.2231	12.13
H(23)	0.4349	0.2132	1.0579	12.13

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

Table 2. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.060(2)	0.055(2)	0.072(2)	-0.004(2)	0.018(2)	-0.023(2)
N(2)	0.051(4)	0.097(5)	0.058(3)	-0.008(3)	-0.006(2)	0.008(3)
C(3)	0.053(5)	0.080(5)	0.049(3)	-0.025(4)	0.009(3)	0.011(3)
C(4)	0.052(4)	0.071(4)	0.055(3)	-0.004(3)	0.013(3)	-0.025(3)
C(5)	0.082(5)	0.054(4)	0.058(3)	-0.012(4)	0.008(3)	-0.012(3)
C(6)	0.041(4)	0.067(4)	0.046(3)	-0.000(3)	-0.002(3)	0.008(3)
C(7)	0.054(4)	0.045(3)	0.047(3)	0.001(3)	0.014(3)	0.020(3)
C(8)	0.041(4)	0.046(3)	0.041(3)	0.001(3)	0.019(2)	0.001(3)
C(9)	0.058(6)	0.059(5)	0.079(4)	-0.009(3)	0.002(3)	0.003(4)
C(10)	0.056(4)	0.072(4)	0.066(3)	0.023(3)	0.010(3)	0.003(3)
C(11)	0.072(5)	0.051(4)	0.050(3)	0.001(3)	0.003(3)	-0.001(3)
C(12)	0.073(5)	0.034(3)	0.071(4)	-0.020(4)	0.018(3)	-0.004(3)
C(13)	0.040(4)	0.059(4)	0.050(3)	-0.002(3)	0.007(3)	-0.003(3)
C(14)	0.054(4)	0.061(4)	0.071(4)	0.004(3)	0.023(3)	-0.005(3)
C(15)	0.075(5)	0.114(6)	0.060(4)	-0.021(4)	0.017(3)	0.011(4)
C(16)	0.059(5)	0.079(5)	0.077(4)	0.020(4)	0.024(3)	0.005(4)
C(17)	0.062(5)	0.078(5)	0.088(4)	-0.006(3)	0.022(4)	0.018(4)
C(18)	0.105(6)	0.110(5)	0.072(4)	0.006(4)	-0.008(3)	0.018(4)
C(19)	0.087(5)	0.118(6)	0.070(4)	-0.018(4)	0.040(4)	-0.041(4)
C(20)	0.057(5)	0.116(6)	0.064(4)	0.015(4)	0.034(3)	0.034(4)
C(21)	0.167(7)	0.069(5)	0.148(6)	-0.024(5)	-0.046(5)	0.049(5)

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(13)	1.451(6)	O(1)	C(19)	1.427(7)
N(2)	C(10)	1.459(6)	N(2)	C(18)	1.441(7)
N(2)	C(21)	1.438(8)	C(3)	C(5)	1.379(9)
C(3)	C(9)	1.362(9)	C(3)	H(4)	0.950
C(4)	C(7)	1.387(7)	C(4)	C(16)	1.373(8)
C(4)	H(5)	0.950	C(5)	C(11)	1.374(8)
C(5)	H(6)	0.950	C(6)	C(10)	1.508(8)
C(6)	C(13)	1.549(7)	C(6)	C(15)	1.517(9)
C(6)	H(3)	0.98(3)	C(7)	C(13)	1.518(8)
C(7)	C(14)	1.406(7)	C(8)	C(11)	1.393(7)
C(8)	C(12)	1.395(8)	C(8)	C(13)	1.539(7)
C(9)	C(12)	1.366(8)	C(9)	H(7)	0.950
C(10)	H(1)	0.950	C(10)	H(2)	0.950
C(11)	H(8)	0.950	C(12)	H(9)	0.950
C(14)	C(17)	1.367(8)	C(14)	H(10)	0.950
C(15)	C(19)	1.544(9)	C(15)	H(14)	0.950
C(15)	H(15)	0.950	C(16)	C(20)	1.388(9)
C(16)	H(11)	0.950	C(17)	C(20)	1.371(9)
C(17)	H(12)	0.950	C(18)	H(18)	0.950
C(18)	H(19)	0.950	C(18)	H(20)	0.950
C(19)	H(16)	0.950	C(19)	H(17)	0.950
C(20)	H(13)	0.950	C(21)	H(21)	0.950
C(21)	H(22)	0.950	C(21)	H(23)	0.950

Table 4. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	O(1)	C(19)	108.3(4)	C(10)	N(2)	C(18)	112.0(4)
C(10)	N(2)	C(21)	112.7(4)	C(18)	N(2)	C(21)	109.9(4)
C(5)	C(3)	C(9)	119.4(5)	C(5)	C(3)	H(4)	120.0
C(9)	C(3)	H(4)	120.6	C(7)	C(4)	C(16)	120.8(5)
C(7)	C(4)	H(5)	119.7	C(16)	C(4)	H(5)	119.5
C(3)	C(5)	C(11)	120.4(5)	C(3)	C(5)	H(6)	117.9
C(11)	C(5)	H(6)	121.7	C(10)	C(6)	C(13)	111.4(5)
C(10)	C(6)	C(15)	113.2(4)	C(10)	C(6)	H(3)	112(2)
C(13)	C(6)	C(15)	100.7(4)	C(13)	C(6)	H(3)	106.4(19)
C(15)	C(6)	H(3)	113(2)	C(4)	C(7)	C(13)	121.0(4)
C(4)	C(7)	C(14)	117.8(5)	C(13)	C(7)	C(14)	121.1(4)
C(11)	C(8)	C(12)	117.6(4)	C(11)	C(8)	C(13)	122.8(5)
C(12)	C(8)	C(13)	119.6(5)	C(3)	C(9)	C(12)	120.9(5)
C(3)	C(9)	H(7)	119.0	C(12)	C(9)	H(7)	120.2
N(2)	C(10)	C(6)	114.2(4)	N(2)	C(10)	H(1)	107.9
N(2)	C(10)	H(2)	109.5	C(6)	C(10)	H(1)	106.6
C(6)	C(10)	H(2)	109.2	H(1)	C(10)	H(2)	109.5
C(5)	C(11)	C(8)	120.7(5)	C(5)	C(11)	H(8)	121.3
C(8)	C(11)	H(8)	118.0	C(8)	C(12)	C(9)	121.0(4)
C(8)	C(12)	H(9)	116.6	C(9)	C(12)	H(9)	122.4
O(1)	C(13)	C(6)	102.2(4)	O(1)	C(13)	C(7)	107.1(4)
O(1)	C(13)	C(8)	109.0(4)	C(6)	C(13)	C(7)	115.5(4)
C(6)	C(13)	C(8)	111.4(4)	C(7)	C(13)	C(8)	111.0(4)
C(7)	C(14)	C(17)	120.1(5)	C(7)	C(14)	H(10)	116.8
C(17)	C(14)	H(10)	123.2	C(6)	C(15)	C(19)	104.0(5)
C(6)	C(15)	H(14)	110.3	C(6)	C(15)	H(15)	110.5
C(19)	C(15)	H(14)	111.9	C(19)	C(15)	H(15)	110.6
H(14)	C(15)	H(15)	109.5	C(4)	C(16)	C(20)	121.2(5)
C(4)	C(16)	H(11)	122.6	C(20)	C(16)	H(11)	116.2
C(14)	C(17)	C(20)	122.3(5)	C(14)	C(17)	H(12)	117.5
C(20)	C(17)	H(12)	120.1	N(2)	C(18)	H(18)	110.0
N(2)	C(18)	H(19)	110.6	N(2)	C(18)	H(20)	107.8
H(18)	C(18)	H(19)	109.5	H(18)	C(18)	H(20)	109.5
H(19)	C(18)	H(20)	109.5	O(1)	C(19)	C(15)	106.5(4)
O(1)	C(19)	H(16)	111.1	O(1)	C(19)	H(17)	109.7
C(15)	C(19)	H(16)	110.9	C(15)	C(19)	H(17)	109.2
H(16)	C(19)	H(17)	109.5	C(16)	C(20)	C(17)	117.7(6)

Table 4. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(16)	C(20)	H(13)	123.4	C(17)	C(20)	H(13)	118.7
N(2)	C(21)	H(21)	109.8	N(2)	C(21)	H(22)	112.0
N(2)	C(21)	H(23)	106.6	H(21)	C(21)	H(22)	109.5
H(21)	C(21)	H(23)	109.5	H(22)	C(21)	H(23)	109.5

Table 5. Torsion Angles(O)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(13)	O(1)	C(19)	C(15)	16.8(4)	C(19)	O(1)	C(13)	C(6)	-37.3(5)
C(19)	O(1)	C(13)	C(7)	-159.2(3)	C(19)	O(1)	C(13)	C(8)	80.7(4)
C(18)	N(2)	C(10)	C(6)	-166.8(5)	C(21)	N(2)	C(10)	C(6)	68.7(6)
C(5)	C(3)	C(9)	C(12)	0.3(8)	C(9)	C(3)	C(5)	C(11)	0.8(9)
C(7)	C(4)	C(16)	C(20)	-1.1(8)	C(16)	C(4)	C(7)	C(13)	179.3(4)
C(16)	C(4)	C(7)	C(14)	1.0(7)	C(3)	C(5)	C(11)	C(8)	-1.5(9)
C(10)	C(6)	C(13)	O(1)	-78.0(5)	C(10)	C(6)	C(13)	C(7)	37.9(6)
C(10)	C(6)	C(13)	C(8)	165.8(4)	C(13)	C(6)	C(10)	N(2)	166.4(4)
C(10)	C(6)	C(15)	C(19)	86.9(5)	C(15)	C(6)	C(10)	N(2)	53.8(6)
C(13)	C(6)	C(15)	C(19)	-32.1(5)	C(15)	C(6)	C(13)	O(1)	42.3(5)
C(15)	C(6)	C(13)	C(7)	158.2(4)	C(15)	C(6)	C(13)	C(8)	-73.9(5)
C(4)	C(7)	C(13)	O(1)	-171.7(4)	C(4)	C(7)	C(13)	C(6)	75.2(5)
C(4)	C(7)	C(13)	C(8)	-52.9(6)	C(4)	C(7)	C(14)	C(17)	-0.9(7)
C(13)	C(7)	C(14)	C(17)	-179.2(4)	C(14)	C(7)	C(13)	O(1)	6.4(6)
C(14)	C(7)	C(13)	C(6)	-106.6(5)	C(14)	C(7)	C(13)	C(8)	125.3(5)
C(11)	C(8)	C(12)	C(9)	-0.0(7)	C(12)	C(8)	C(11)	C(5)	1.1(8)
C(11)	C(8)	C(13)	O(1)	-161.3(4)	C(11)	C(8)	C(13)	C(6)	-49.3(7)
C(11)	C(8)	C(13)	C(7)	81.0(6)	C(13)	C(8)	C(11)	C(5)	-175.7(5)
C(12)	C(8)	C(13)	O(1)	21.9(6)	C(12)	C(8)	C(13)	C(6)	133.9(5)
C(12)	C(8)	C(13)	C(7)	-95.8(6)	C(13)	C(8)	C(12)	C(9)	176.9(5)
C(3)	C(9)	C(12)	C(8)	-0.7(9)	C(7)	C(14)	C(17)	C(20)	0.9(8)
C(6)	C(15)	C(19)	O(1)	11.1(5)	C(4)	C(16)	C(20)	C(17)	1.0(8)
C(14)	C(17)	C(20)	C(16)	-0.9(8)					

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(3)[1)]	3.01(3)	O(1)	H(8)[1)]	3.102
O(1)	H(21)[1)]	3.080	O(1)	H(23)[1)]	3.373
N(2)	H(11)[2)]	3.055	C(3)	C(19)[3)]	3.520(8)
C(3)	H(6)[4)]	3.263	C(3)	H(16)[3)]	2.951
C(3)	H(17)[3)]	3.301	C(4)	H(4)[4)]	3.131
C(4)	H(6)[4)]	3.469	C(4)	H(7)[5)]	3.232
C(4)	H(12)[6)]	3.392	C(5)	C(9)[5)]	3.484(9)
C(5)	C(12)[5)]	3.549(8)	C(5)	H(6)[4)]	3.353
C(5)	H(7)[6)]	3.512	C(5)	H(9)[6)]	2.975
C(5)	H(16)[3)]	3.400	C(5)	H(17)[3)]	3.204
C(6)	H(10)[6)]	3.489	C(7)	H(4)[4)]	3.134
C(8)	H(6)[4)]	3.349	C(8)	H(17)[3)]	3.563
C(9)	C(5)[4)]	3.484(9)	C(9)	H(5)[4)]	3.367
C(9)	H(6)[1)]	3.120	C(9)	H(6)[4)]	3.200
C(9)	H(14)[7)]	3.202	C(9)	H(15)[7)]	3.289
C(9)	H(16)[3)]	3.246	C(9)	H(17)[3)]	3.510
C(11)	H(6)[4)]	3.407	C(11)	H(9)[6)]	3.066
C(11)	H(17)[3)]	3.322	C(12)	C(5)[4)]	3.549(8)
C(12)	H(6)[1)]	3.008	C(12)	H(6)[4)]	3.233
C(12)	H(8)[1)]	3.495	C(12)	H(14)[7)]	3.101
C(14)	H(3)[1)]	3.56(3)	C(14)	H(4)[4)]	3.032
C(14)	H(5)[1)]	3.340	C(14)	H(8)[1)]	3.432
C(14)	H(23)[1)]	3.262	C(15)	H(7)[3)]	3.189
C(15)	H(9)[3)]	3.496	C(16)	H(4)[4)]	3.069
C(16)	H(7)[5)]	3.386	C(16)	H(12)[6)]	3.416
C(16)	H(15)[8)]	3.421	C(16)	H(18)[9)]	3.462
C(16)	H(19)[8)]	3.375	C(16)	H(19)[9)]	3.273
C(17)	H(4)[4)]	2.964	C(17)	H(5)[1)]	3.341
C(17)	H(20)[9)]	3.421	C(18)	C(20)[9)]	3.583(8)
C(18)	H(2)[9)]	3.568	C(18)	H(11)[2)]	3.281
C(18)	H(12)[10)]	3.473	C(18)	H(13)[2)]	3.364
C(19)	C(3)[7)]	3.520(8)	C(19)	H(21)[1)]	3.045
C(20)	C(18)[9)]	3.583(8)	C(20)	H(4)[4)]	2.991
C(20)	H(19)[8)]	3.388	C(20)	H(19)[9)]	3.209
C(20)	H(20)[9)]	3.292	C(21)	H(1)[6)]	3.225
C(21)	H(10)[6)]	3.302	C(21)	H(13)[11)]	3.592
C(21)	H(16)[6)]	3.210	C(21)	H(20)[6)]	3.583

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

atom	atom	distance	atom	atom	distance
H(1)	C(21)[1)]	3.225	H(1)	H(21)[1)]	3.013
H(1)	H(22)[1)]	3.216	H(1)	H(23)[1)]	2.912
H(2)	C(18)[9)]	3.568	H(2)	H(10)[6)]	3.242
H(2)	H(18)[9)]	2.807	H(2)	H(20)[9)]	3.488
H(3)	O(1)[6)]	3.01(3)	H(3)	C(14)[6)]	3.56(3)
H(3)	H(10)[6)]	2.654	H(3)	H(16)[6)]	3.487
H(4)	C(4)[5)]	3.131	H(4)	C(7)[5)]	3.134
H(4)	C(14)[5)]	3.032	H(4)	C(16)[5)]	3.069
H(4)	C(17)[5)]	2.964	H(4)	C(20)[5)]	2.991
H(4)	H(5)[4)]	3.369	H(4)	H(8)[4)]	3.526
H(4)	H(10)[5)]	3.540	H(4)	H(12)[5)]	3.505
H(4)	H(13)[5)]	3.438	H(4)	H(16)[3)]	2.985
H(5)	C(9)[5)]	3.367	H(5)	C(14)[6)]	3.340
H(5)	C(17)[6)]	3.341	H(5)	H(4)[5)]	3.369
H(5)	H(6)[4)]	3.442	H(5)	H(7)[5)]	2.720
H(5)	H(10)[6)]	3.005	H(5)	H(12)[6)]	3.021
H(6)	C(3)[5)]	3.263	H(6)	C(4)[5)]	3.469
H(6)	C(5)[5)]	3.353	H(6)	C(8)[5)]	3.349
H(6)	C(9)[6)]	3.120	H(6)	C(9)[5)]	3.200
H(6)	C(11)[5)]	3.407	H(6)	C(12)[6)]	3.008
H(6)	C(12)[5)]	3.233	H(6)	H(5)[5)]	3.442
H(6)	H(7)[6)]	2.703	H(6)	H(9)[6)]	2.487
H(6)	H(15)[3)]	3.549	H(6)	H(17)[3)]	3.599
H(7)	C(4)[4)]	3.232	H(7)	C(5)[1)]	3.512
H(7)	C(15)[7)]	3.189	H(7)	C(16)[4)]	3.386
H(7)	H(5)[4)]	2.720	H(7)	H(6)[1)]	2.703
H(7)	H(8)[4)]	3.553	H(7)	H(11)[4)]	3.062
H(7)	H(14)[7)]	2.914	H(7)	H(15)[7)]	2.605
H(7)	H(16)[3)]	3.470	H(8)	O(1)[6)]	3.102
H(8)	C(12)[6)]	3.495	H(8)	C(14)[6)]	3.432
H(8)	H(4)[5)]	3.526	H(8)	H(7)[5)]	3.553
H(8)	H(9)[6)]	2.648	H(8)	H(10)[6)]	2.913
H(9)	C(5)[1)]	2.975	H(9)	C(11)[1)]	3.066
H(9)	C(15)[7)]	3.496	H(9)	H(6)[1)]	2.487
H(9)	H(8)[1)]	2.648	H(9)	H(14)[7)]	2.764
H(9)	H(15)[7)]	3.518	H(10)	C(6)[1)]	3.489
H(10)	C(21)[1)]	3.302	H(10)	H(2)[1)]	3.242

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

atom	atom	distance	atom	atom	distance
H(10)	H(3)[1)]	2.654	H(10)	H(4)[4)]	3.540
H(10)	H(5)[1)]	3.005	H(10)	H(8)[1)]	2.913
H(10)	H(21)[1)]	3.304	H(10)	H(23)[1)]	2.504
H(11)	N(2)[8)]	3.055	H(11)	C(18)[8)]	3.281
H(11)	H(7)[5)]	3.062	H(11)	H(12)[6)]	3.089
H(11)	H(15)[8)]	2.892	H(11)	H(19)[8)]	2.716
H(11)	H(19)[9)]	3.225	H(11)	H(21)[8)]	3.577
H(12)	C(4)[1)]	3.392	H(12)	C(16)[1)]	3.416
H(12)	C(18)[12)]	3.473	H(12)	H(4)[4)]	3.505
H(12)	H(5)[1)]	3.021	H(12)	H(11)[1)]	3.089
H(12)	H(18)[12)]	2.799	H(12)	H(19)[12)]	3.305
H(12)	H(20)[9)]	3.598	H(12)	H(22)[12)]	3.008
H(13)	C(18)[8)]	3.364	H(13)	C(21)[13)]	3.592
H(13)	H(4)[4)]	3.438	H(13)	H(13)[14)]	3.122
H(13)	H(19)[8)]	2.870	H(13)	H(19)[9)]	3.247
H(13)	H(20)[8)]	3.136	H(13)	H(20)[9)]	3.513
H(13)	H(21)[13)]	3.348	H(13)	H(22)[13)]	2.961
H(14)	C(9)[3)]	3.202	H(14)	C(12)[3)]	3.101
H(14)	H(7)[3)]	2.914	H(14)	H(9)[3)]	2.764
H(14)	H(17)[3)]	2.861	H(15)	C(9)[3)]	3.289
H(15)	C(16)[2)]	3.421	H(15)	H(6)[7)]	3.549
H(15)	H(7)[3)]	2.605	H(15)	H(9)[3)]	3.518
H(15)	H(11)[2)]	2.892	H(16)	C(3)[7)]	2.951
H(16)	C(5)[7)]	3.400	H(16)	C(9)[7)]	3.246
H(16)	C(21)[1)]	3.210	H(16)	H(3)[1)]	3.487
H(16)	H(4)[7)]	2.985	H(16)	H(7)[7)]	3.470
H(16)	H(21)[1)]	2.311	H(16)	H(23)[1)]	3.446
H(17)	C(3)[7)]	3.301	H(17)	C(5)[7)]	3.204
H(17)	C(8)[7)]	3.563	H(17)	C(9)[7)]	3.510
H(17)	C(11)[7)]	3.322	H(17)	H(6)[7)]	3.599
H(17)	H(14)[7)]	2.861	H(18)	C(16)[9)]	3.462
H(18)	H(2)[9)]	2.807	H(18)	H(12)[10)]	2.799
H(19)	C(16)[2)]	3.375	H(19)	C(16)[9)]	3.273
H(19)	C(20)[2)]	3.388	H(19)	C(20)[9)]	3.209
H(19)	H(11)[2)]	2.716	H(19)	H(11)[9)]	3.225
H(19)	H(12)[10)]	3.305	H(19)	H(13)[2)]	2.870
H(19)	H(13)[9)]	3.247	H(19)	H(19)[15)]	2.991

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

atom	atom	distance	atom	atom	distance
H(20)	C(17)[9]	3.421	H(20)	C(20)[9]	3.292
H(20)	C(21)[1]	3.583	H(20)	H(2)[9]	3.488
H(20)	H(12)[9]	3.598	H(20)	H(13)[2]	3.136
H(20)	H(13)[9]	3.513	H(20)	H(22)[1]	2.990
H(20)	H(23)[1]	3.539	H(21)	O(1)[6]	3.080
H(21)	C(19)[6]	3.045	H(21)	H(1)[6]	3.013
H(21)	H(10)[6]	3.304	H(21)	H(11)[2]	3.577
H(21)	H(13)[11]	3.348	H(21)	H(16)[6]	2.311
H(22)	H(1)[6]	3.216	H(22)	H(12)[10]	3.008
H(22)	H(13)[11]	2.961	H(22)	H(20)[6]	2.990
H(23)	O(1)[6]	3.373	H(23)	C(14)[6]	3.262
H(23)	H(1)[6]	2.912	H(23)	H(10)[6]	2.504
H(23)	H(16)[6]	3.446	H(23)	H(20)[6]	3.539

Symmetry Operators:

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

Absolute configuration analysis

	H	K	L	Fo diff	Fc diff	Fc diff/sigma
Correct trend:	5	-1	0	-0.49	-0.15	-0.30
Incorrect:	-1	-1	3	0.65	-0.28	-0.28
Incorrect:	-1	-1	3	0.05	-0.28	-0.26
Incorrect:	-1	-1	3	1.46	-0.28	-0.25
Correct trend:	-1	-1	3	-0.58	-0.28	-0.24
Incorrect:	-9	-1	1	-1.19	0.21	0.23
Correct trend:	-1	-1	3	-1.90	-0.28	-0.23
Correct trend:	5	-1	0	-0.66	-0.15	-0.22
Correct trend:	-1	-1	3	-0.57	-0.28	-0.21
Correct trend:	-1	-1	3	-0.21	-0.28	-0.21
Correct trend:	-4	-2	2	-0.99	-0.23	-0.21
Incorrect:	-1	-1	3	0.47	-0.28	-0.21
Incorrect:	0	-2	1	0.19	-0.20	-0.20
Correct trend:	-9	-1	1	0.05	0.21	0.20
Incorrect:	-4	-2	2	0.20	-0.23	-0.20
Correct trend:	-1	-1	3	-0.94	-0.28	-0.20

Correct trend:	-4	-2	2	-0.06	-0.23	-0.20
Incorrect:	-9	-1	1	-0.63	0.21	0.19
Correct trend:	0	-2	1	-2.01	-0.20	-0.19
Incorrect:	0	-2	1	0.70	-0.20	-0.19
Incorrect:	0	-2	1	0.32	-0.20	-0.19
Incorrect:	-1	-1	3	0.35	-0.28	-0.19
Correct trend:	7	-1	0	0.91	0.24	0.19
Correct trend:	9	-1	1	1.10	0.15	0.19
Correct trend:	-9	-1	1	1.19	0.21	0.19
Incorrect:	0	-2	1	0.93	-0.20	-0.18
Correct trend:	-4	-2	1	1.05	0.18	0.18
Correct trend:	0	-2	1	-1.10	-0.20	-0.18
Correct trend:	-9	-1	1	1.09	0.21	0.18
Correct trend:	5	-1	0	-0.39	-0.15	-0.18
Correct trend:	5	-1	0	-0.93	-0.15	-0.18
Incorrect:	5	-1	0	2.55	-0.15	-0.18
Incorrect:	5	-1	0	0.02	-0.15	-0.17
Correct trend:	-9	-1	1	0.90	0.21	0.17
Correct trend:	7	-1	0	0.32	0.24	0.17
Incorrect:	-4	-2	2	0.47	-0.23	-0.17
Correct trend:	-5	-1	3	1.50	0.17	0.16
Incorrect:	-4	-2	1	-0.21	0.18	0.16
Correct trend:	0	-2	1	-1.17	-0.20	-0.16
Correct trend:	-9	-1	1	1.07	0.21	0.16
Incorrect:	-9	-1	1	-0.31	0.21	0.16
Incorrect:	5	-1	0	0.09	-0.15	-0.16
Incorrect:	-4	-2	2	0.92	-0.23	-0.16
Correct trend:	-4	-2	2	-1.13	-0.23	-0.16
Correct trend:	0	-2	1	-0.21	-0.20	-0.16
Correct trend:	-4	-2	2	-0.42	-0.23	-0.15
Correct trend:	-9	-1	1	1.22	0.21	0.15
Correct trend:	-9	-1	1	0.14	0.21	0.15
Correct trend:	-4	-2	2	-0.19	-0.23	-0.15
Incorrect:	4	-2	2	-1.33	0.15	0.15
Incorrect:	-5	-1	3	-1.29	0.17	0.15
Correct trend:	-5	-1	3	0.73	0.17	0.15
Correct trend:	-4	-2	1	0.09	0.18	0.14
Correct trend:	-4	-2	1	0.05	0.18	0.14
Incorrect:	7	-1	0	-2.50	0.24	0.14
Correct trend:	7	-1	0	1.67	0.24	0.14
Correct trend:	-4	-2	2	-0.31	-0.23	-0.14
Correct trend:	9	-1	1	0.36	0.15	0.13
Correct trend:	-5	-1	3	0.73	0.17	0.13
Correct trend:	4	-2	2	0.15	0.15	0.13
Incorrect:	9	-1	1	-0.48	0.15	0.13
Correct trend:	3	-1	2	0.61	0.11	0.13
Correct trend:	9	-1	0	-0.38	-0.10	-0.13
Incorrect:	3	-1	2	-0.71	0.11	0.13
Correct trend:	3	-1	2	1.94	0.11	0.13
Incorrect:	7	-1	0	-3.61	0.24	0.13
Correct trend:	-4	-2	1	0.03	0.18	0.13
Incorrect:	-5	-1	3	-0.99	0.17	0.13
Incorrect:	7	-1	0	-0.22	0.24	0.13
Incorrect:	-4	-2	2	1.38	-0.23	-0.13
Correct trend:	3	-1	2	0.68	0.11	0.12
Correct trend:	-5	-1	3	1.23	0.17	0.12

Correct trend:	-5	-1	3	0.03	0.17	0.12
Correct trend:	4	-2	2	2.83	0.15	0.12
Incorrect:	-4	-2	1	-0.28	0.18	0.12
Correct trend:	3	-1	2	0.09	0.11	0.12
Incorrect:	9	-1	0	0.79	-0.10	-0.12
Correct trend:	7	-1	2	0.29	0.12	0.12
Incorrect:	9	-1	1	-2.41	0.15	0.12
Correct trend:	5	-1	3	-1.02	-0.14	-0.12
Correct trend:	7	-1	0	1.36	0.24	0.11
Correct trend:	9	-1	1	0.73	0.15	0.11
Incorrect:	5	-1	3	1.68	-0.14	-0.11
Incorrect:	3	-1	2	-0.71	0.11	0.11
Correct trend:	9	-1	1	1.07	0.15	0.11
Incorrect:	-8	-2	2	0.16	-0.14	-0.11
Incorrect:	-13	-1	2	-0.93	0.10	0.11
Incorrect:	-4	-2	1	-1.68	0.18	0.11
Incorrect:	-5	-1	3	-0.71	0.17	0.11
Correct trend:	5	-1	3	-1.82	-0.14	-0.11
Correct trend:	-5	-1	3	2.79	0.17	0.11
Correct trend:	9	-1	1	0.50	0.15	0.11
Incorrect:	-10	-2	1	0.58	-0.15	-0.11
Correct trend:	-10	-2	1	-0.46	-0.15	-0.10
Correct trend:	3	-1	2	0.23	0.11	0.10
Correct trend:	9	-1	1	1.34	0.15	0.10
Incorrect:	9	-1	1	-0.79	0.15	0.10
Correct trend:	3	-1	2	0.65	0.11	0.10
Incorrect:	2	-2	1	2.60	-0.08	-0.10
Incorrect:	-5	-1	3	-0.64	0.17	0.10
Incorrect:	4	-2	2	-1.44	0.15	0.10
Correct trend:	5	-1	3	-2.54	-0.14	-0.10
Incorrect:	5	-1	3	0.56	-0.14	-0.10
Incorrect:	-8	-2	2	1.33	-0.14	-0.10
Incorrect:	9	-1	0	0.44	-0.10	-0.10
Correct trend:	-13	-1	3	-2.71	-0.13	-0.10
Correct trend:	4	-2	2	2.60	0.15	0.10
Incorrect:	-4	-2	3	0.33	-0.13	-0.09
Correct trend:	4	-2	2	3.12	0.15	0.09
Incorrect:	4	-2	2	-1.18	0.15	0.09
Correct trend:	-13	-1	2	0.10	0.10	0.09
Correct trend:	-8	-2	2	-0.38	-0.14	-0.09
Incorrect:	9	-1	0	0.82	-0.10	-0.09
Correct trend:	3	-3	0	-0.25	-0.15	-0.09
Incorrect:	9	-1	0	0.43	-0.10	-0.09
Incorrect:	-13	-1	3	1.97	-0.13	-0.09
Correct trend:	4	-2	2	3.64	0.15	0.09
Incorrect:	-13	-1	3	1.99	-0.13	-0.09
Incorrect:	4	-2	2	-0.18	0.15	0.09
Correct trend:	-11	-1	1	-2.82	-0.08	-0.09
Correct trend:	-13	-1	2	0.49	0.10	0.09
Incorrect:	7	-1	2	-1.97	0.12	0.09
Incorrect:	-7	-3	2	5.44	-0.16	-0.09
Correct trend:	11	-1	2	8.03	0.17	0.09
Incorrect:	-1	-1	4	-0.68	0.11	0.09
Incorrect:	-8	-2	2	1.36	-0.14	-0.09
Incorrect:	3	-1	2	-0.73	0.11	0.09
Incorrect:	-10	-2	1	0.90	-0.15	-0.09

Incorrect:	2	-2	2	0.39	-0.10	-0.09
Incorrect:	5	-1	1	-0.27	0.15	0.09
Incorrect:	-10	-2	1	4.65	-0.15	-0.09
Incorrect:	4	-2	3	-0.63	0.13	0.08
Correct trend:	-13	-1	1	-2.12	-0.09	-0.08
Incorrect:	3	-3	0	1.68	-0.15	-0.08
Correct trend:	7	-1	2	3.00	0.12	0.08
Incorrect:	8	-2	1	-0.33	0.15	0.08
Incorrect:	3	-3	2	-1.98	0.11	0.08
Incorrect:	2	-2	1	1.26	-0.08	-0.08
Correct trend:	5	-1	3	-0.37	-0.14	-0.08
Incorrect:	-8	-2	2	0.06	-0.14	-0.08
Incorrect:	-8	-2	2	2.55	-0.14	-0.08
Correct trend:	-4	-2	3	-0.95	-0.13	-0.08
Incorrect:	-4	-2	3	2.55	-0.13	-0.08
Correct trend:	8	-2	1	1.28	0.15	0.08
Correct trend:	-7	-3	2	-0.88	-0.16	-0.08
Incorrect:	7	-1	2	-2.42	0.12	0.08
Incorrect:	-1	-1	4	-1.73	0.11	0.08
Correct trend:	7	-1	2	4.05	0.12	0.08
Incorrect:	5	-1	1	-0.96	0.15	0.08
Correct trend:	-4	-2	3	-1.70	-0.13	-0.08
Incorrect:	7	-1	4	-2.60	0.11	0.08
Correct trend:	5	-1	3	-0.44	-0.14	-0.08
Incorrect:	2	-2	2	0.12	-0.10	-0.08
Correct trend:	4	-2	3	4.71	0.13	0.08
Incorrect:	5	-1	1	-2.14	0.15	0.08
Correct trend:	6	-2	1	0.27	0.07	0.08
Incorrect:	9	-1	0	2.22	-0.10	-0.08
Incorrect:	3	-1	0	-0.72	0.18	0.08
Correct trend:	5	-1	1	1.68	0.15	0.08
Correct trend:	-4	-2	3	-0.58	-0.13	-0.08
Incorrect:	7	-1	2	-0.32	0.12	0.07
Incorrect:	5	-1	3	0.11	-0.14	-0.07
Correct trend:	5	-1	1	1.65	0.15	0.07
Correct trend:	-8	-2	2	-2.36	-0.14	-0.07
Incorrect:	3	-3	0	1.71	-0.15	-0.07
Correct trend:	8	-2	1	3.03	0.15	0.07
Incorrect:	2	-2	1	1.24	-0.08	-0.07
Incorrect:	-13	-1	3	0.86	-0.13	-0.07
Incorrect:	9	-1	0	0.90	-0.10	-0.07
Incorrect:	-13	-1	2	-1.58	0.10	0.07
Incorrect:	11	-1	2	-1.67	0.17	0.07
Correct trend:	9	-1	0	-0.88	-0.10	-0.07
Correct trend:	-4	-2	3	-2.48	-0.13	-0.07
Correct trend:	3	-3	0	-0.96	-0.15	-0.07
Correct trend:	-8	-2	2	-0.70	-0.14	-0.07
Correct trend:	5	-1	1	2.19	0.15	0.07
Incorrect:	-7	-3	2	1.11	-0.16	-0.07
Incorrect:	-4	-2	3	2.73	-0.13	-0.07
Incorrect:	-1	-1	4	-0.23	0.11	0.07
Incorrect:	-8	-2	2	2.01	-0.14	-0.07
Incorrect:	5	-1	1	-1.44	0.15	0.07
Correct trend:	2	-2	1	-1.31	-0.08	-0.07
Incorrect:	8	-2	1	-1.99	0.15	0.07
Correct trend:	8	-2	1	1.06	0.15	0.07

Incorrect:	3	-3	2	-1.30	0.11	0.07
Correct trend:	5	-1	1	2.16	0.15	0.07
Incorrect:	-7	-1	1	2.98	-0.08	-0.07
Incorrect:	2	-2	1	0.72	-0.08	-0.07
Correct trend:	-13	-1	3	-4.97	-0.13	-0.07
Correct trend:	-11	-1	1	-1.65	-0.08	-0.07
Incorrect:	3	-3	0	0.65	-0.15	-0.07
Correct trend:	-4	-2	3	-0.46	-0.13	-0.07
Correct trend:	-13	-1	1	-1.84	-0.09	-0.07
Incorrect:	-13	-1	1	1.23	-0.09	-0.07
Correct trend:	2	-2	1	-1.12	-0.08	-0.07
Correct trend:	8	-2	1	0.88	0.15	0.07
Incorrect:	1	-1	4	4.87	-0.12	-0.07
Incorrect:	-16	-2	2	-1.21	0.10	0.07
Incorrect:	-1	-1	1	-0.97	0.20	0.07
Correct trend:	-1	-1	1	0.20	0.20	0.07

Summary	Total	Sum delta(Fc)	<average>
Number of reflections processed:	4829		
Fc difference agrees with Fo:	793	53.100	0.067
Fc difference disagrees with Fo:	784	49.530	0.063
F(H)=F(-H) reflexions:	332		
Reflections without Friedel mates:	1010		
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:	793	0	0	0	0	0
Incorrect:	784	0	0	0	0	0

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