Sample: SU032

X-ray Structure Report

for

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Friday, June 04, 2010

DISCUSSION

The compound crystallizes as colorless, blade-like crystals grown from a heptane solution. There are two molecules of the compound in the unit cell of the primitive, acentric, monoclinic space group $P2_1$. The absolute configuration was determined both by the known handedness of the molecule and by comparison of intensities of Friedel pairs of reflections (Flack parameter = 0.000(7), a value of zero indicates the correct absolute configuration, a value of one the inverted absolute stereochemistry).

The structure of the molecule and stereochemistry is as expected. The vinyl group was found to be disordered by an approximately 180° rotation about the C-C single bond. The occupancies of the pairs of disordered carbons were refined and summed to unity giving a nearly 0.6:0.4 occupancy ratio. The thermal displacement parameters on the major and minor components were refined isotropically, while the atoms in the core of the molecule were refined with anisotropic thermal motion parameters. Inclusion of this disorder model improved the overall model. The disorder results in a slight shortening of the C-C bond distance to the minor component (C4-C12A = 1.467(11) Å compared with C4-C12 = 1.565(8) Å). However, it does not alter the characterization of the species.

The remaining bond distances and angles are otherwise as would be expected.

CRYSTAL SUMMARY

Crystal data for $C_{24}H_{25}BrO_6$; M_r = 489.35; monoclinic; space group $P2_1$; a = 6.8101(6) Å; b = 13.0126(10) Å; c = 12.8280(10) Å; α = 90°; β = 93.991(2)°; γ = 90°; V = 1134.02(16) $Å^3$; Z = 2; T = 100(2) K; λ(Mo-Kα) = 0.71073 Å; μ(Mo-Kα) = 1.849 mm^{-1}; d_{calc} = 1.433g.cm^{-3}; 12969 reflections collected; 4446 unique (R_{int} = 0.0493); giving R_1 = 0.0360, wR_2 = 0.0578 for 3643 data with [I>2σ(I)] and R_1 = 0.0514, wR_2 = 0.0627 for all 4446 data. Residual electron density ($e^-.Å^{-3}$) max/min: 0.295/-0.270.

An arbitrary sphere of data were collected on a colorless blade-like crystal, having approximate dimensions of 0.29 × 0.16 × 0.13 mm, on a Bruker Kappa X8-APEX-II diffractometer using a combination of ω- and φ-scans of 0.5°. Data were corrected for absorption and polarization effects and analyzed for space group determination. The structure was solved by direct methods and expanded routinely. The model was refined by full-matrix least-squares analysis of F^2 against all reflections. All non-hydrogen atoms were refined with anisotropic thermal displacement parameters. Unless otherwise noted, hydrogen atoms were included in calculated positions. Thermal parameters for the hydrogens were tied to the isotropic thermal parameter of the atom to which they are bonded (1.5 × for methyl, 1.2 × for all others).

Table 1. Crystal data and structure refinement for su032.

Identification code	su032
Empirical formula	$C_{24}H_{25}BrO_6$
Formula weight	489.35
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 6.8101(6) Å α = 90°
	b = 13.0126(10) Å β = 93.991(2)°
	c = 12.8280(10) Å γ = 90°
Volume	1134.02(16) $Å^3$
Z	2
Density (calculated)	1.433 $g.cm^{-3}$
Absorption coefficient (μ)	1.849 mm^{-1}
F(000)	504
Crystal size	0.29 × 0.16 × 0.13 mm^3
θ range for data collection	1.59 to 26.44°
Index ranges	$-8 \le h \le 8$, $-16 \le k \le 16$, $-15 \le l \le 15$
Reflections collected	12969
Independent reflections	4446 [R_{int} = 0.0493]
Completeness to θ = 26.44°	97.9 %
Absorption correction	empirical
Max. and min. transmission	0.7950 and 0.6161
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4446 / 1 / 282
Goodness-of-fit on F^2	0.906
Final R indices [I>2σ(I)]	R_1 = 0.0360, wR_2 = 0.0578
R indices (all data)	R_1 = 0.0514, wR_2 = 0.0627
Absolute structure parameter	0.000(7)
Largest diff. peak and hole	0.295 and -0.270 $e^-.Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for su032. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	0.68616(4)	0.39252(3)	1.46914(2)	0.027(1)
O(1)	0.1761(4)	0.4901(2)	0.6345(2)	0.029(1)
O(2)	0.2802(3)	0.54803(17)	0.79734(17)	0.026(1)
O(3)	0.1793(3)	0.46063(16)	0.99772(16)	0.021(1)
O(4)	-0.0678(3)	0.3970(3)	1.08558(15)	0.032(1)
O(5)	0.5029(3)	0.3772(2)	0.79942(16)	0.029(1)
O(6)	0.2711(3)	0.28825(16)	0.87739(17)	0.021(1)
C(1)	0.1830(5)	0.4543(2)	0.8125(3)	0.022(1)
C(2)	0.0628(6)	0.4343(3)	0.7047(3)	0.023(1)
C(3)	0.2548(6)	0.5792(3)	0.6879(3)	0.030(1)
C(4)	0.0484(5)	0.4604(3)	0.9027(2)	0.026(1)
C(5)	0.1002(5)	0.4232(2)	1.0836(3)	0.022(1)
C(6)	0.2495(4)	0.4190(2)	1.1749(2)	0.017(1)
C(7)	0.4482(5)	0.4395(2)	1.1661(3)	0.022(1)
C(8)	0.5789(5)	0.4331(2)	1.2548(3)	0.022(1)
C(9)	0.5070(4)	0.4061(3)	1.3490(2)	0.021(1)
C(10)	0.3117(4)	0.3862(4)	1.3587(2)	0.023(1)
C(11)	0.1827(4)	0.3928(4)	1.2707(2)	0.021(1)
C(12)	-0.0500(10)	0.5691(6)	0.9001(5)	0.023(2)
C(13)	-0.2388(10)	0.5765(5)	0.8793(5)	0.034(2)
C(12A)	-0.1131(15)	0.5352(8)	0.8981(7)	0.023(3)
C(13A)	-0.0761(14)	0.6301(8)	0.9278(7)	0.034(3)
C(14)	0.3402(5)	0.3701(3)	0.8295(2)	0.022(1)
C(15)	0.4008(5)	0.1989(2)	0.8847(3)	0.026(1)
C(16)	0.5660(5)	0.2118(3)	0.9694(3)	0.036(1)
C(17)	0.0434(6)	0.3248(3)	0.6702(3)	0.023(1)
C(18)	0.1926(6)	0.2752(3)	0.6205(3)	0.023(1)
C(19)	0.1718(5)	0.1737(3)	0.5902(3)	0.027(1)
C(20)	0.0040(6)	0.1192(3)	0.6097(3)	0.030(1)
C(21)	-0.1434(5)	0.1673(3)	0.6609(3)	0.030(1)
C(22)	-0.1254(5)	0.2696(3)	0.6903(3)	0.026(1)
C(23)	0.4533(6)	0.6030(3)	0.6484(3)	0.037(1)
C(24)	0.1120(6)	0.6692(3)	0.6784(3)	0.036(1)
H(2A)	-0.0708	0.4659	0.7060	0.028
H(4A)	-0.0501	0.4033	0.9014	0.032
H(7A)	0.4946	0.4576	1.1004	0.026
H(8A)	0.7150	0.4471	1.2503	0.027
H(10A)	0.2657	0.3684	1.4246	0.027
H(11A)	0.0467	0.3791	1.2762	0.026
H(12A)	0.0274	0.6290	0.9136	0.027
H(13A)	-0.3153	0.5163	0.8659	0.041

H(13B)	-0.3003	0.6420	0.8775	0.041
H(12B)	-0.2426	0.5152	0.8740	0.027
H(13C)	0.0538	0.6495	0.9518	0.041
H(13D)	-0.1791	0.6795	0.9253	0.041
H(15A)	0.4580	0.1881	0.8167	0.031
H(15B)	0.3229	0.1371	0.8999	0.031
H(16A)	0.6353	0.1463	0.9805	0.054
H(16B)	0.5109	0.2333	1.0345	0.054
H(16C)	0.6583	0.2642	0.9478	0.054
H(18A)	0.3093	0.3115	0.6074	0.028
H(19A)	0.2738	0.1411	0.5555	0.033
H(20A)	-0.0102	0.0495	0.5883	0.036
H(21A)	-0.2578	0.1299	0.6760	0.036
H(22A)	-0.2283	0.3022	0.7242	0.031
H(23A)	0.5403	0.5435	0.6599	0.056
H(23B)	0.5109	0.6625	0.6862	0.056
H(23C)	0.4378	0.6186	0.5736	0.056
H(24A)	-0.0175	0.6469	0.6985	0.054
H(24B)	0.1009	0.6937	0.6060	0.054
H(24C)	0.1608	0.7249	0.7247	0.054

Table 3. Anisotropic displacement parameters ($Å^2$) for su032.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	0.0301(2)	0.0298(2)	0.0195(2)	0.0005(2)	-0.0056(1)	0.0026(2)
O(1)	0.051(2)	0.0192(16)	0.0160(15)	0.0033(12)	0.0058(13)	0.0072(13)
O(2)	0.0383(15)	0.0216(14)	0.0190(14)	0.0035(11)	0.0008(11)	0.0059(11)
O(3)	0.0236(12)	0.0285(13)	0.0096(12)	0.0015(10)	-0.0004(10)	0.0009(10)
O(4)	0.0224(11)	0.0544(15)	0.0206(11)	0.0004(18)	0.0006(9)	-0.0096(19)
O(5)	0.0284(12)	0.0279(18)	0.0328(13)	0.0067(14)	0.0126(10)	0.0072(13)
O(6)	0.0213(12)	0.0222(13)	0.0188(13)	0.0051(11)	0.0020(10)	0.0067(10)
C(1)	0.0279(19)	0.023(2)	0.0159(19)	0.0028(15)	0.0015(16)	0.0088(16)
C(2)	0.028(2)	0.028(2)	0.014(2)	0.0027(15)	0.0050(17)	0.0099(16)
C(3)	0.046(2)	0.025(2)	0.019(2)	0.0041(16)	0.0043(18)	0.0077(18)
C(4)	0.0218(18)	0.044(2)	0.0129(19)	-0.0008(16)	-0.0009(15)	0.0137(16)
C(5)	0.0265(18)	0.024(2)	0.0159(18)	-0.0025(14)	0.0020(15)	-0.0037(14)
C(6)	0.0219(16)	0.014(2)	0.0140(17)	-0.0008(12)	0.0000(13)	0.0012(12)
C(7)	0.0229(18)	0.0261(19)	0.0171(19)	0.0006(15)	0.0043(15)	-0.0024(14)
C(8)	0.0177(16)	0.026(2)	0.024(2)	0.0020(14)	0.0025(15)	-0.0012(13)
C(9)	0.0250(16)	0.019(2)	0.0177(16)	-0.0008(18)	-0.0028(13)	0.0019(18)
C(10)	0.0270(15)	0.0259(18)	0.0152(15)	0.004(2)	0.0049(12)	0.002(2)
C(11)	0.0205(14)	0.0223(16)	0.0217(16)	0.007(2)	0.0036(12)	0.004(2)
C(14)	0.0294(18)	0.021(3)	0.0152(17)	0.0024(15)	0.0040(15)	0.0057(16)
C(15)	0.032(2)	0.017(2)	0.030(2)	0.0044(16)	0.0015(17)	0.0101(15)
C(16)	0.026(2)	0.030(2)	0.051(3)	0.0115(19)	-0.0050(19)	0.0034(17)
C(17)	0.031(2)	0.028(2)	0.009(2)	0.0050(16)	0.0007(17)	0.0115(18)
C(18)	0.027(2)	0.024(2)	0.019(2)	0.0026(18)	0.0035(17)	0.0034(17)
C(19)	0.032(2)	0.031(2)	0.020(2)	0.0018(17)	0.0109(17)	0.0088(17)
C(20)	0.042(2)	0.024(2)	0.024(2)	0.0011(17)	0.0028(18)	0.0049(18)
C(21)	0.029(2)	0.034(2)	0.026(2)	0.0039(18)	0.0039(17)	0.0038(17)
C(22)	0.0260(19)	0.035(2)	0.018(2)	0.0026(17)	0.0029(16)	0.0122(17)
C(23)	0.053(3)	0.027(2)	0.034(2)	0.0088(18)	0.014(2)	0.0082(19)
C(24)	0.053(3)	0.025(2)	0.030(2)	0.0064(18)	0.000(2)	0.0119(19)

Table 4. Bond lengths [Å] for su032.

atom-atom	distance	atom-atom	distance
Br(1)-C(9)	1.906(3)	O(1)-C(2)	1.425(4)
O(1)-C(3)	1.432(4)	O(2)-C(1)	1.408(4)
O(2)-C(3)	1.460(4)	O(3)-C(5)	1.350(4)
O(3)-C(4)	1.459(3)	O(4)-C(5)	1.196(4)
O(5)-C(14)	1.202(4)	O(6)-C(14)	1.332(4)
O(6)-C(15)	1.459(4)	C(1)-C(4)	1.527(4)
C(1)-C(14)	1.536(4)	C(1)-C(2)	1.578(5)
C(2)-C(17)	1.495(5)	C(2)-H(2A)	1.0000
C(3)-C(23)	1.508(5)	C(3)-C(24)	1.521(5)
C(4)-C(12A)	1.467(11)	C(4)-C(12)	1.565(8)
C(4)-H(4A)	1.0000	C(5)-C(6)	1.498(4)
C(6)-C(11)	1.383(4)	C(6)-C(7)	1.391(4)
C(7)-C(8)	1.398(4)	C(7)-H(7A)	0.9500
C(8)-C(9)	1.380(4)	C(8)-H(8A)	0.9500
C(9)-C(10)	1.370(4)	C(10)-C(11)	1.384(3)
C(10)-H(10A)	0.9500	C(11)-H(11A)	0.9500
C(12)-C(13)	1.298(10)	C(12)-H(12A)	0.9500
C(13)-H(13A)	0.9500	C(13)-H(13B)	0.9500
C(12A)-C(13A)	1.312(15)	C(12A)-H(12B)	0.9500
C(13A)-H(13C)	0.9500	C(13A)-H(13D)	0.9500
C(15)-C(16)	1.517(4)	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800
C(17)-C(22)	1.394(5)	C(17)-C(18)	1.395(5)
C(18)-C(19)	1.381(5)	C(18)-H(18A)	0.9500
C(19)-C(20)	1.383(5)	C(19)-H(19A)	0.9500
C(20)-C(21)	1.387(5)	C(20)-H(20A)	0.9500
C(21)-C(22)	1.387(5)	C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500	C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800	C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800		

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for su032.

atom-atom-atom	angle	atom-atom-atom	angle
C(2)-O(1)-C(3)	108.1(3)	C(1)-O(2)-C(3)	110.4(2)
C(5)-O(3)-C(4)	115.2(2)	C(14)-O(6)-C(15)	115.8(3)
O(2)-C(1)-C(4)	111.8(3)	O(2)-C(1)-C(14)	107.9(3)
C(4)-C(1)-C(14)	112.3(3)	O(2)-C(1)-C(2)	104.0(3)
C(4)-C(1)-C(2)	111.8(3)	C(14)-C(1)-C(2)	108.7(3)
O(1)-C(2)-C(17)	109.9(3)	O(1)-C(2)-C(1)	101.5(3)
C(17)-C(2)-C(1)	116.5(3)	O(1)-C(2)-H(2A)	109.5
C(17)-C(2)-H(2A)	109.5	C(1)-C(2)-H(2A)	109.5
O(1)-C(3)-O(2)	104.5(3)	O(1)-C(3)-C(23)	108.7(3)
O(2)-C(3)-C(23)	109.3(3)	O(1)-C(3)-C(24)	111.7(3)
O(2)-C(3)-C(24)	108.8(3)	C(23)-C(3)-C(24)	113.4(3)
O(3)-C(4)-C(12A)	116.4(4)	O(3)-C(4)-C(1)	105.6(3)
C(12A)-C(4)-C(1)	119.5(4)	O(3)-C(4)-C(12)	104.6(3)
C(12A)-C(4)-C(12)	23.1(4)	C(1)-C(4)-C(12)	108.0(3)
O(3)-C(4)-H(4A)	112.7	C(12A)-C(4)-H(4A)	89.5
C(1)-C(4)-H(4A)	112.7	C(12)-C(4)-H(4A)	112.7
O(4)-C(5)-O(3)	123.9(3)	O(4)-C(5)-C(6)	124.8(3)
O(3)-C(5)-C(6)	111.3(3)	C(11)-C(6)-C(7)	120.1(3)
C(11)-C(6)-C(5)	117.1(3)	C(7)-C(6)-C(5)	122.7(3)
C(6)-C(7)-C(8)	119.4(3)	C(6)-C(7)-H(7A)	120.3
C(8)-C(7)-H(7A)	120.3	C(9)-C(8)-C(7)	118.9(3)
C(9)-C(8)-H(8A)	120.5	C(7)-C(8)-H(8A)	120.5
C(10)-C(9)-C(8)	122.3(3)	C(10)-C(9)-Br(1)	118.7(2)
C(8)-C(9)-Br(1)	119.0(2)	C(9)-C(10)-C(11)	118.7(3)
C(9)-C(10)-H(10A)	120.7	C(11)-C(10)-H(10A)	120.7
C(6)-C(11)-C(10)	120.7(3)	C(6)-C(11)-H(11A)	119.7
C(10)-C(11)-H(11A)	119.7	C(13)-C(12)-C(4)	119.1(7)
C(13)-C(12)-H(12A)	120.4	C(4)-C(12)-H(12A)	120.4
C(12)-C(13)-H(13A)	120.0	C(12)-C(13)-H(13B)	120.0
H(13A)-C(13)-H(13B)	120.0	C(13A)-C(12A)-C(4)	119.0(9)
C(13A)-C(12A)-H(12B)	120.5	C(4)-C(12A)-H(12B)	120.5
C(12A)-C(13A)-H(13C)	120.0	C(12A)-C(13A)-H(13D)	120.0
H(13C)-C(13A)-H(13D)	120.0	O(5)-C(14)-O(6)	124.9(3)
O(5)-C(14)-C(1)	123.3(3)	O(6)-C(14)-C(1)	111.7(3)
O(6)-C(15)-C(16)	111.9(3)	O(6)-C(15)-H(15A)	109.2
C(16)-C(15)-H(15A)	109.2	O(6)-C(15)-H(15B)	109.2
C(16)-C(15)-H(15B)	109.2	H(15A)-C(15)-H(15B)	107.9
C(15)-C(16)-H(16A)	109.5	C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5	C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(16B)-C(16)-H(16C)	109.5
C(22)-C(17)-C(18)	118.9(4)	C(22)-C(17)-C(2)	119.5(3)
C(18)-C(17)-C(2)	121.6(4)	C(19)-C(18)-C(17)	120.5(4)

C(19)-C(18)-H(18A)	119.7	C(17)-C(18)-H(18A)	119.7
C(18)-C(19)-C(20)	120.6(3)	C(18)-C(19)-H(19A)	119.7
C(20)-C(19)-H(19A)	119.7	C(19)-C(20)-C(21)	119.3(3)
C(19)-C(20)-H(20A)	120.4	C(21)-C(20)-H(20A)	120.4
C(22)-C(21)-C(20)	120.6(3)	C(22)-C(21)-H(21A)	119.7
C(20)-C(21)-H(21A)	119.7	C(21)-C(22)-C(17)	120.2(3)
C(21)-C(22)-H(22A)	119.9	C(17)-C(22)-H(22A)	119.9
C(3)-C(23)-H(23A)	109.5	C(3)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5	C(3)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(3)-C(24)-H(24A)	109.5	C(3)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(3)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for su032.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C(3)-O(2)-C(1)-C(4)	-129.0(3)	C(3)-O(2)-C(1)-C(14)	107.1(3)
C(3)-O(2)-C(1)-C(2)	-8.2(3)	C(3)-O(1)-C(2)-C(17)	-158.2(3)
C(3)-O(1)-C(2)-C(1)	-34.4(3)	O(2)-C(1)-C(2)-O(1)	25.6(3)
C(4)-C(1)-C(2)-O(1)	146.4(3)	C(14)-C(1)-C(2)-O(1)	-89.2(3)
O(2)-C(1)-C(2)-C(17)	144.9(3)	C(4)-C(1)-C(2)-C(17)	-94.4(4)
C(14)-C(1)-C(2)-C(17)	30.1(5)	C(2)-O(1)-C(3)-O(2)	30.3(4)
C(2)-O(1)-C(3)-C(23)	146.9(3)	C(2)-O(1)-C(3)-C(24)	-87.2(3)
C(1)-O(2)-C(3)-O(1)	-12.3(3)	C(1)-O(2)-C(3)-C(23)	-128.4(3)
C(1)-O(2)-C(3)-C(24)	107.1(3)	C(5)-O(3)-C(4)-C(12A)	71.4(6)
C(5)-O(3)-C(4)-C(1)	-153.4(3)	C(5)-O(3)-C(4)-C(12)	92.7(4)
O(2)-C(1)-C(4)-O(3)	-73.6(3)	C(14)-C(1)-C(4)-O(3)	47.8(4)
C(2)-C(1)-C(4)-O(3)	170.3(3)	O(2)-C(1)-C(4)-C(12A)	59.9(6)
C(14)-C(1)-C(4)-C(12A)	-178.6(5)	C(2)-C(1)-C(4)-C(12A)	-56.2(6)
O(2)-C(1)-C(4)-C(12)	37.9(4)	C(14)-C(1)-C(4)-C(12)	159.3(4)
C(2)-C(1)-C(4)-C(12)	-78.3(4)	C(4)-O(3)-C(5)-O(4)	-4.3(5)
C(4)-O(3)-C(5)-C(6)	175.6(2)	O(4)-C(5)-C(6)-C(11)	-6.9(5)
O(3)-C(5)-C(6)-C(11)	173.1(3)	O(4)-C(5)-C(6)-C(7)	172.6(4)
O(3)-C(5)-C(6)-C(7)	-7.3(4)	C(11)-C(6)-C(7)-C(8)	0.1(5)
C(5)-C(6)-C(7)-C(8)	-179.5(3)	C(6)-C(7)-C(8)-C(9)	0.3(5)
C(7)-C(8)-C(9)-C(10)	-0.6(6)	C(7)-C(8)-C(9)-Br(1)	177.8(2)
C(8)-C(9)-C(10)-C(11)	0.5(7)	Br(1)-C(9)-C(10)-C(11)	-177.9(4)
C(7)-C(6)-C(11)-C(10)	-0.2(6)	C(5)-C(6)-C(11)-C(10)	179.4(4)
C(9)-C(10)-C(11)-C(6)	-0.1(7)	O(3)-C(4)-C(12)-C(13)	-134.0(5)
C(12A)-C(4)-C(12)-C(13)	-9.9(10)	C(1)-C(4)-C(12)-C(13)	113.8(6)
O(3)-C(4)-C(12A)-C(13A)	45.0(10)	C(1)-C(4)-C(12A)-C(13A)	-83.8(9)
C(12)-C(4)-C(12A)-C(13A)	-18.4(9)	C(15)-O(6)-C(14)-O(5)	-5.3(5)
C(15)-O(6)-C(14)-C(1)	172.2(2)	O(2)-C(1)-C(14)-O(5)	-23.0(4)
C(4)-C(1)-C(14)-O(5)	-146.7(3)	C(2)-C(1)-C(14)-O(5)	89.2(4)
O(2)-C(1)-C(14)-O(6)	159.4(2)	C(4)-C(1)-C(14)-O(6)	35.7(4)
C(2)-C(1)-C(14)-O(6)	-88.4(3)	C(14)-O(6)-C(15)-C(16)	76.9(4)
O(1)-C(2)-C(17)-C(22)	-149.0(3)	C(1)-C(2)-C(17)-C(22)	96.4(4)
O(1)-C(2)-C(17)-C(18)	32.7(5)	C(1)-C(2)-C(17)-C(18)	-82.0(4)
C(22)-C(17)-C(18)-C(19)	1.1(6)	C(2)-C(17)-C(18)-C(19)	179.5(3)
C(17)-C(18)-C(19)-C(20)	-0.8(6)	C(18)-C(19)-C(20)-C(21)	-0.4(5)
C(19)-C(20)-C(21)-C(22)	1.4(5)	C(20)-C(21)-C(22)-C(17)	-1.2(5)
C(18)-C(17)-C(22)-C(21)	-0.1(5)	C(2)-C(17)-C(22)-C(21)	-178.5(3)

Symmetry transformations used to generate equivalent atoms:

checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: su032

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=6.8101(6) b=13.0126(10) c=12.828(1)
alpha=90 beta=93.991(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1134.02(16)	1134.02(16)
Space group	P 21	P21
Hall group	P 2yb	P 2yb
Moiety formula	C24 H25 Br O6	C24 H25 Br O6
Sum formula	C24 H25 Br O6	C24 H25 Br O6
Mr	489.34	489.35
Dx,g cm-3	1.433	1.433
Z	2	2
Mu (mm-1)	1.849	1.849
F000	504.0	504.0
F000'	503.67	
h,k,lmax	8,16,16	8,16,15
Nref	2448[4680]	4446
Tmin,Tmax	0.708,0.786	0.616,0.795
Tmin'	0.579	

Correction method= EMPIRICAL

Data completeness= 1.82/0.95 Theta(max)= 26.440

R(reflections)= 0.0360(3643) wR2(reflections)= 0.0627(4446)

S = 0.906 Npar= 282

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 2

Alert level C
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.98

Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max          26.44
          From the CIF: _reflns_number_total              4446
          Count of symmetry unique reflns         2448
          Completeness (_total/calc)           181.62%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      1998
          Fraction of Friedel pairs measured     0.816
          Are heavy atom types Z>Si present        yes
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      6.00 Perc.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......     23.10 Deg.
             C12A -C4   -C12     1.555   1.555   1.555
PLAT791_ALERT_4_G Note: The Model has Chirality at C1     (Verify)         R
PLAT791_ALERT_4_G Note: The Model has Chirality at C2     (Verify)         S
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..      0.01
```

```
   0 ALERT level A = In general: serious problem
   1 ALERT level B = Potentially serious problem
   1 ALERT level C = Check and explain
   6 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Publication of your CIF in IUCr journals

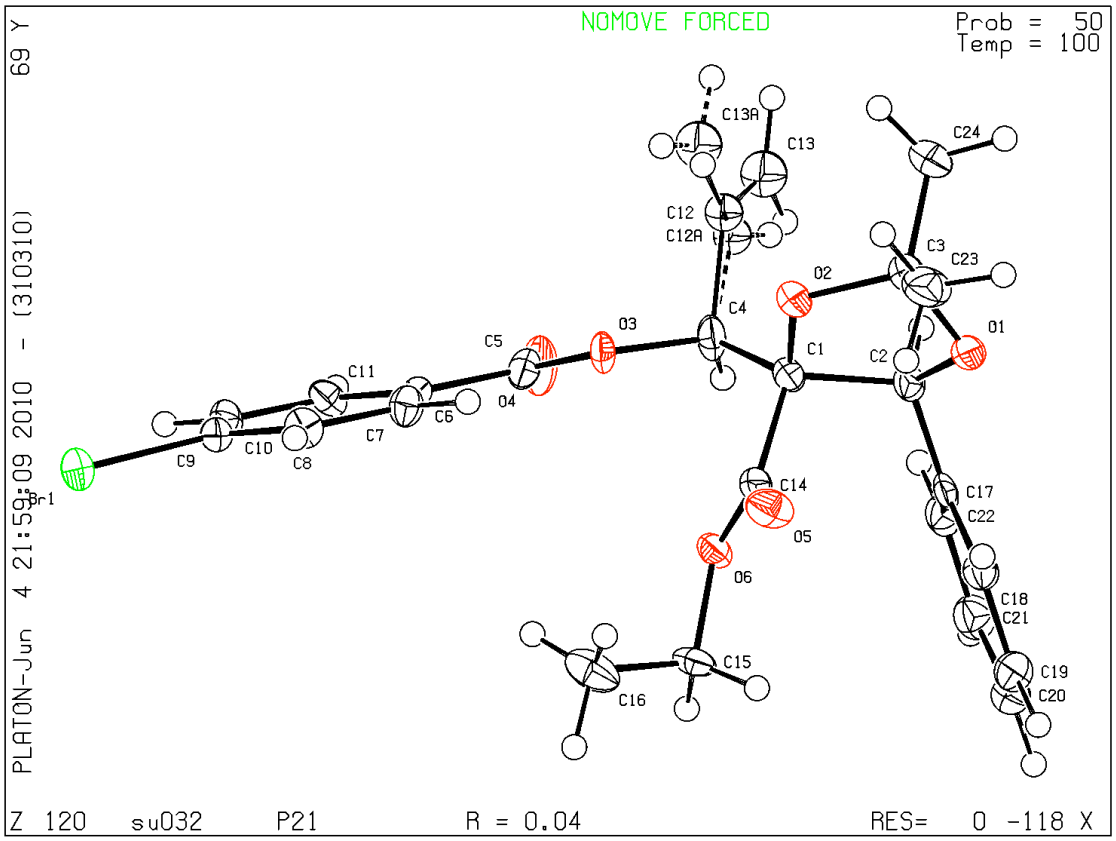
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

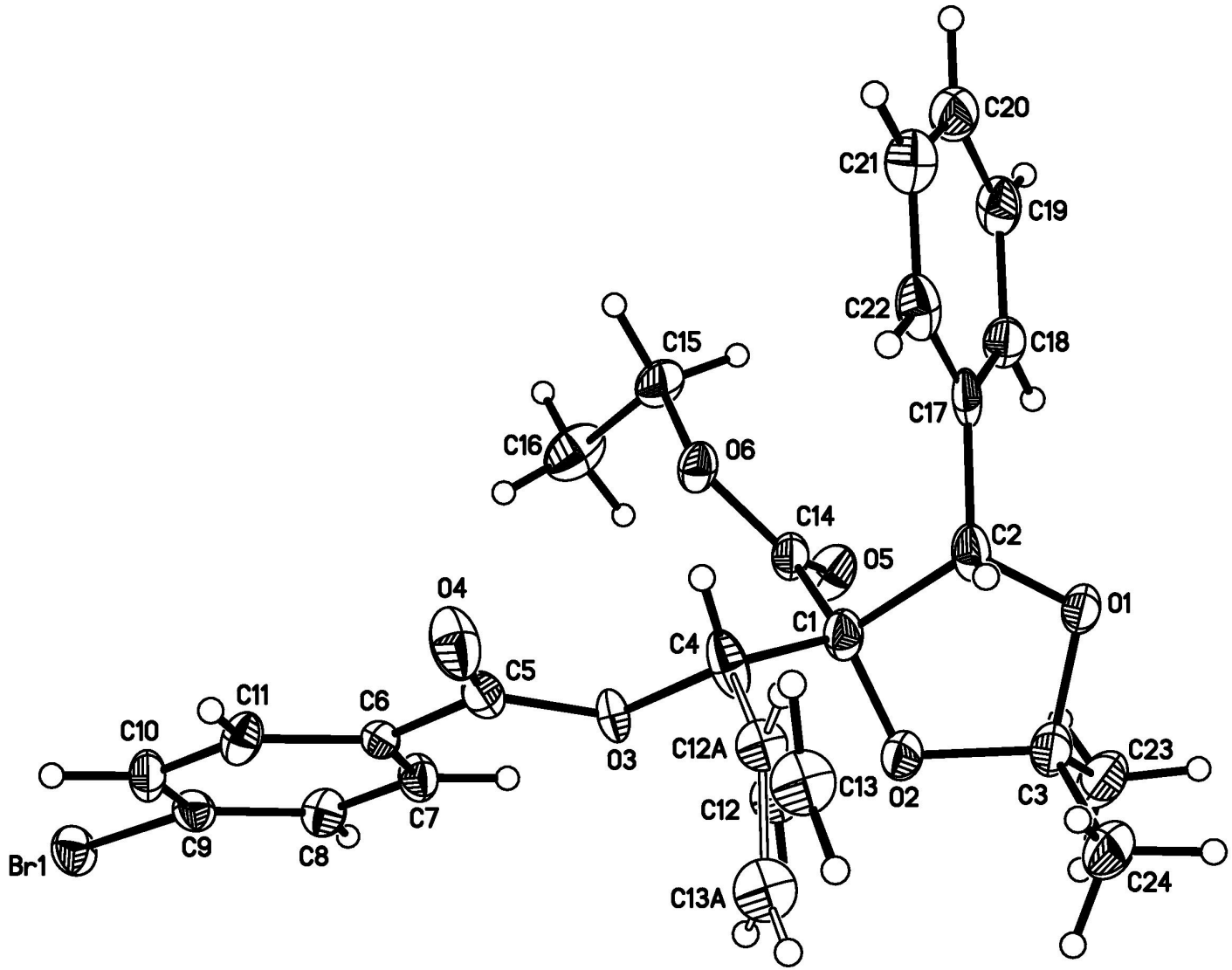
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 31/03/2010; check.def file version of 22/03/2010

Datablock su032 - ellipsoid plot

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C22
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C15
C16
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C14
O5
C2
O1
O4
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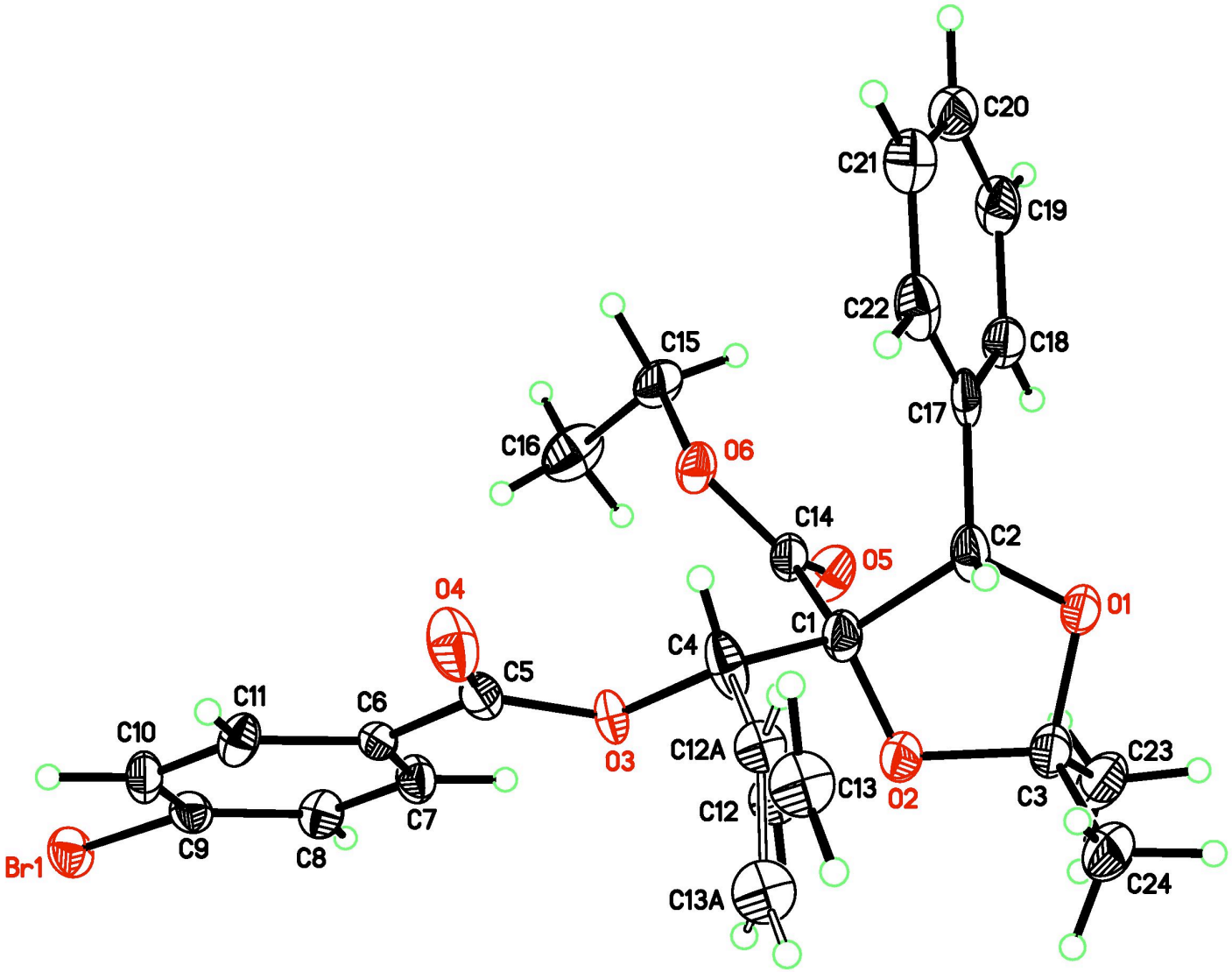
C4
C5
C11
C6
C10
O3
C12A
C23
C13
O2
C3
C12
C7
C9
C8
Br1
C13A
C24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O5
O4
C1
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C5
C11
C6
C10
O3
C12A
C23
C13
O2
C3
C12
C7
C9
C8
Br1
C24
C13A