APPENDIX 7

X-ray Crystallography Reports

Relevant to Chapter 4

A7.1 CRYSTAL STRUCTURE ANALYSIS FOR COMPOUND 117

The *mixture of diastereomers* **117** were recrystallized from *i*-PrOH/heptane (liquid/liquid diffusion) to provide crystals suitable for X-ray analysis. *NOTE: Crystallographic data have been deposited in the Cambridge Database (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number CCDC* 959511.

Figure A7.1.1. *ORTEP drawing of* ***117****.*

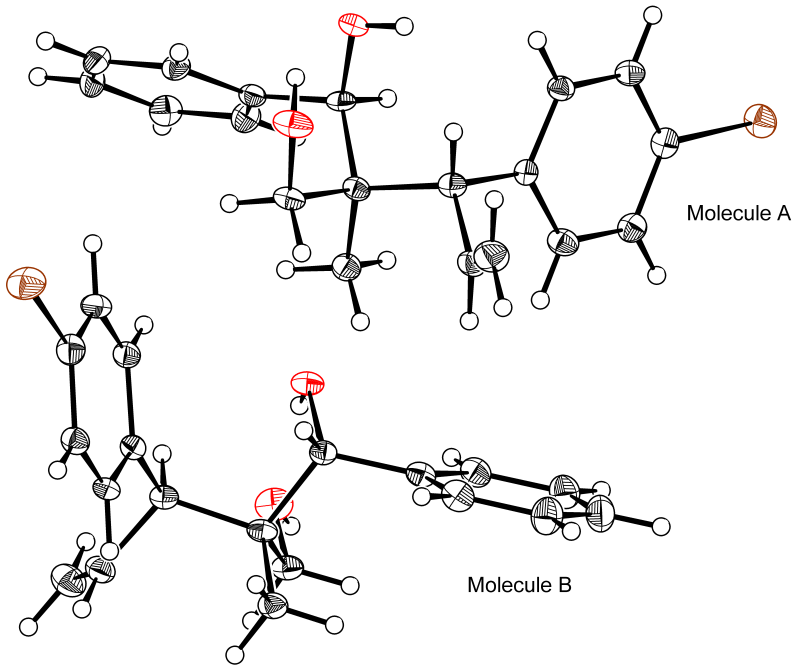

Table A7.1*. Crystal Data and Structure Analysis Details for diol* ***117****.*

Empirical formula	C19 H21 Br O2
Formula weight	361.27
Crystallization solvent	*i*-PrOH/heptane
Crystal shape	plate
Crystal color	colourless
Crystal size	0.06 x 0.16 x 0.45 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker APEX-II CCD	
Wavelength	0.71073 Å MoK	
Data collection temperature	100 K	
Theta range for 9925 reflections used in lattice determination	2.31 to 24.19°	
Unit cell dimensions	a = 11.871(3) Å b = 13.179(3) Å c = 21.761(5) Å	⟨= 90° ®= 90° © = 90°
Volume	3404.5(13) Å^3	

Z	8
Crystal system	orthorhombic
Space group	P 21 21 21 (# 19)
Density (calculated)	1.410 g/cm^3
F(000)	1488
Theta range for data collection	1.8 to 32.3°
Completeness to theta = 25.000°	99.8%
Index ranges	-17 ″ h ″ 17, -19 ″ k ″ 19, -32 ″ l ″ 32
Data collection scan type	and scans
Reflections collected	88198
Independent reflections	11569 [R_{int}= 0.1174]
Reflections > 2 ∫(I)	8213
Average ∫(I)/(net I)	0.0905
Absorption coefficient	2.42 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.6406

Structure Solution and Refinement

Primary solution method	dual
Secondary solution method	?
Hydrogen placement	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11569 / 0 / 403
Treatment of hydrogen atoms	constr
Goodness-of-fit on F^2	1.31
Final R indices [I>2 ∫(I), 8213 reflections]	R1 = 0.0549, wR2 = 0.1052
R indices (all data)	R1 = 0.0967, wR2 = 0.1137
Type of weighting scheme used	calc
Weighting scheme used	w=1/[^2^(Fo^2^)+(0.0300P)^2^] where
P=(Fo^2^+2Fc^2^)/3	
Max shift/error	0.000
Average shift/error	0.000
Absolute structure parameter	0.032(5)
Extinction coefficient	n/a
Largest diff. peak and hole	1.70 and -0.98 e·Å^{-3}

	Programs Used
Cell refinement	SAINT V8.32B (Bruker-AXS, 2007)
Data collection	APEX2 2013.6-2 (Bruker-AXS, 2007)
Data reduction	SAINT V8.32B (Bruker-AXS, 2007)
Structure solution	SHELXT (Sheldrick, 2012)
Structure refinement	SHELXL-2013/2 (Sheldrick, 2013)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Table A7.2. *Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for* ***117***. *U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.*

	x	y	z	U_{eq}
Br(1)	6018(1)	702(1)	2623(1)	24(1)
Br(1B)	2988(1)	6376(1)	6793(1)	29(1)
O(1)	2594(3)	2303(2)	5173(1)	17(1)
O(1B)	7801(3)	4619(2)	5244(2)	18(1)
O(2B)	9886(3)	5315(3)	5428(2)	24(1)
O(2)	1686(3)	4120(3)	5230(2)	24(1)
C(12)	4092(4)	2845(3)	5863(2)	16(1)
C(18)	2777(4)	4578(3)	5206(2)	18(1)
C(9)	3015(5)	4701(4)	3852(2)	18(1)
C(18B)	9487(4)	6230(4)	5137(2)	19(1)
C(8B)	6117(4)	7301(3)	6134(2)	17(1)
C(2B)	8002(4)	6397(4)	5956(2)	15(1)
C(1B)	8221(4)	6404(4)	5243(2)	16(1)
C(1)	3608(4)	3879(3)	4879(2)	15(1)
C(15)	4893(5)	2837(4)	7069(2)	24(1)
C(14)	3765(4)	3049(4)	6953(2)	22(1)
C(11)	3668(4)	2816(4)	5202(2)	16(1)
C(6)	5187(4)	1642(4)	3110(2)	18(1)
C(17)	5219(4)	2643(4)	5991(2)	21(1)
C(2)	3195(4)	3711(4)	4194(2)	16(1)
C(7B)	4982(4)	7302(4)	6324(2)	18(1)
C(8)	4928(4)	3307(4)	3522(2)	20(1)
C(3)	3933(4)	2995(3)	3819(2)	14(1)
C(13)	3366(4)	3055(4)	6356(2)	17(1)
C(19B)	7923(4)	7429(4)	4952(2)	19(1)
C(12B)	7652(4)	5450(4)	4243(2)	18(1)
C(6B)	4508(4)	6393(4)	6517(2)	21(1)
C(19)	4775(4)	4374(4)	4898(2)	20(1)
C(16)	5615(4)	2644(4)	6592(2)	22(1)
C(11B)	7514(4)	5552(3)	4936(2)	15(1)
C(4)	3595(4)	1989(4)	3747(2)	16(1)
C(5)	4218(4)	1308(4)	3397(2)	19(1)
C(3B)	6758(4)	6422(4)	6135(2)	15(1)
C(9B)	8651(4)	7213(4)	6288(2)	21(1)

C(7)	5550(4)	2637(4)	3168(2)	19(1)
C(13B)	8529(4)	4866(4)	3986(2)	22(1)
C(14B)	8635(5)	4779(4)	3355(2)	25(1)
C(4B)	6236(4)	5523(4)	6338(2)	18(1)
C(10B)	9604(4)	7033(4)	6590(2)	27(1)
C(10)	2036(5)	4974(4)	3618(2)	27(1)
C(15B)	7867(5)	5270(4)	2970(2)	28(1)
C(17B)	6896(4)	5927(4)	3852(2)	22(1)
C(5B)	5122(4)	5503(4)	6526(2)	21(1)
C(16B)	7008(5)	5844(4)	3217(2)	28(1)

Table A7.3. *Bond lengths [Å] and angles [°] for* ***117***.

Br(1)-C(6)	1.906(5)
Br(1B)-C(6B)	1.902(5)
O(1)-H(1)	0.8400
O(1)-C(11)	1.445(5)
O(1B)-H(1B)	0.8400
O(1B)-C(11B)	1.443(5)
O(2B)-H(2B)	0.8400
O(2B)-C(18B)	1.442(6)
O(2)-H(2)	0.8400
O(2)-C(18)	1.430(5)
C(12)-C(11)	1.525(6)
C(12)-C(17)	1.391(7)
C(12)-C(13)	1.404(6)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(18)-C(1)	1.527(6)
C(9)-H(9)	0.9500
C(9)-C(2)	1.517(6)
C(9)-C(10)	1.319(7)
C(18B)-H(18C)	0.9900
C(18B)-H(18D)	0.9900
C(18B)-C(1B)	1.538(6)
C(8B)-H(8B)	0.9500
C(8B)-C(7B)	1.409(7)
C(8B)-C(3B)	1.386(7)
C(2B)-H(2BA)	1.0000
C(2B)-C(1B)	1.574(6)
C(2B)-C(3B)	1.527(6)
C(2B)-C(9B)	1.507(7)
C(1B)-C(19B)	1.532(6)
C(1B)-C(11B)	1.553(6)
C(1)-C(11)	1.568(6)
C(1)-C(2)	1.585(6)
C(1)-C(19)	1.531(6)
C(15)-H(15)	0.9500
C(15)-C(14)	1.391(7)
C(15)-C(16)	1.369(7)
C(14)-H(14)	0.9500

C(14)-C(13)	1.382(7)
C(11)-H(11)	1.0000
C(6)-C(5)	1.381(7)
C(6)-C(7)	1.386(7)
C(17)-H(17)	0.9500
C(17)-C(16)	1.391(6)
C(2)-H(2A)	1.0000
C(2)-C(3)	1.524(6)
C(7B)-H(7B)	0.9500
C(7B)-C(6B)	1.389(7)
C(8)-H(8)	0.9500
C(8)-C(3)	1.408(6)
C(8)-C(7)	1.385(7)
C(3)-C(4)	1.394(7)
C(13)-H(13)	0.9500
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(12B)-C(11B)	1.522(6)
C(12B)-C(13B)	1.411(7)
C(12B)-C(17B)	1.387(7)
C(6B)-C(5B)	1.381(7)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(16)-H(16)	0.9500
C(11B)-H(11B)	1.0000
C(4)-H(4)	0.9500
C(4)-C(5)	1.391(7)
C(5)-H(5)	0.9500
C(3B)-C(4B)	1.408(7)
C(9B)-H(9B)	0.9500
C(9B)-C(10B)	1.329(7)
C(7)-H(7)	0.9500
C(13B)-H(13B)	0.9500
C(13B)-C(14B)	1.384(7)
C(14B)-H(14B)	0.9500
C(14B)-C(15B)	1.398(8)
C(4B)-H(4B)	0.9500
C(4B)-C(5B)	1.385(7)
C(10B)-H(10C)	0.9500
C(10B)-H(10D)	0.9500
C(10)-H(10A)	0.9500
C(10)-H(10B)	0.9500
C(15B)-H(15B)	0.9500
C(15B)-C(16B)	1.379(8)
C(17B)-H(17B)	0.9500
C(17B)-C(16B)	1.392(7)
C(5B)-H(5B)	0.9500
C(16B)-H(16B)	0.9500

C(11)-O(1)-H(1)	109.5

C(11B)-O(1B)-H(1B)	109.5
C(18B)-O(2B)-H(2B)	109.5
C(18)-O(2)-H(2)	109.5
C(17)-C(12)-C(11)	120.1(4)
C(17)-C(12)-C(13)	118.4(4)
C(13)-C(12)-C(11)	121.5(4)
O(2)-C(18)-H(18A)	109.6
O(2)-C(18)-H(18B)	109.6
O(2)-C(18)-C(1)	110.3(4)
H(18A)-C(18)-H(18B)	108.1
C(1)-C(18)-H(18A)	109.6
C(1)-C(18)-H(18B)	109.6
C(2)-C(9)-H(9)	118.4
C(10)-C(9)-H(9)	118.4
C(10)-C(9)-C(2)	123.3(5)
O(2B)-C(18B)-H(18C)	109.1
O(2B)-C(18B)-H(18D)	109.1
O(2B)-C(18B)-C(1B)	112.3(4)
H(18C)-C(18B)-H(18D)	107.9
C(1B)-C(18B)-H(18C)	109.1
C(1B)-C(18B)-H(18D)	109.1
C(7B)-C(8B)-H(8B)	119.2
C(3B)-C(8B)-H(8B)	119.2
C(3B)-C(8B)-C(7B)	121.7(4)
C(1B)-C(2B)-H(2BA)	106.1
C(3B)-C(2B)-H(2BA)	106.1
C(3B)-C(2B)-C(1B)	114.3(3)
C(9B)-C(2B)-H(2BA)	106.1
C(9B)-C(2B)-C(1B)	112.5(4)
C(9B)-C(2B)-C(3B)	110.9(4)
C(18B)-C(1B)-C(2B)	108.0(4)
C(18B)-C(1B)-C(11B)	110.8(4)
C(19B)-C(1B)-C(18B)	107.2(4)
C(19B)-C(1B)-C(2B)	112.0(4)
C(19B)-C(1B)-C(11B)	109.6(4)
C(11B)-C(1B)-C(2B)	109.3(4)
C(18)-C(1)-C(11)	111.0(4)
C(18)-C(1)-C(2)	108.8(4)
C(18)-C(1)-C(19)	108.3(4)
C(11)-C(1)-C(2)	108.1(4)
C(19)-C(1)-C(11)	109.2(4)
C(19)-C(1)-C(2)	111.4(4)
C(14)-C(15)-H(15)	119.9
C(16)-C(15)-H(15)	119.9
C(16)-C(15)-C(14)	120.2(4)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-C(15)	120.1(4)
C(13)-C(14)-H(14)	120.0
O(1)-C(11)-C(12)	110.2(4)
O(1)-C(11)-C(1)	111.0(3)
O(1)-C(11)-H(11)	106.9
C(12)-C(11)-C(1)	114.5(4)

C(12)-C(11)-H(11)	106.9
C(1)-C(11)-H(11)	106.9
C(5)-C(6)-Br(1)	118.3(4)
C(5)-C(6)-C(7)	121.3(4)
C(7)-C(6)-Br(1)	120.4(4)
C(12)-C(17)-H(17)	119.6
C(12)-C(17)-C(16)	120.8(4)
C(16)-C(17)-H(17)	119.6
C(9)-C(2)-C(1)	112.6(4)
C(9)-C(2)-H(2A)	106.2
C(9)-C(2)-C(3)	110.5(4)
C(1)-C(2)-H(2A)	106.2
C(3)-C(2)-C(1)	114.3(4)
C(3)-C(2)-H(2A)	106.2
C(8B)-C(7B)-H(7B)	120.8
C(6B)-C(7B)-C(8B)	118.4(4)
C(6B)-C(7B)-H(7B)	120.8
C(3)-C(8)-H(8)	119.4
C(7)-C(8)-H(8)	119.4
C(7)-C(8)-C(3)	121.1(4)
C(8)-C(3)-C(2)	123.2(4)
C(4)-C(3)-C(2)	118.9(4)
C(4)-C(3)-C(8)	117.8(4)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-C(12)	120.4(4)
C(14)-C(13)-H(13)	119.8
C(1B)-C(19B)-H(19D)	109.5
C(1B)-C(19B)-H(19E)	109.5
C(1B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(13B)-C(12B)-C(11B)	121.4(4)
C(17B)-C(12B)-C(11B)	119.9(4)
C(17B)-C(12B)-C(13B)	118.8(4)
C(7B)-C(6B)-Br(1B)	119.3(4)
C(5B)-C(6B)-Br(1B)	119.1(4)
C(5B)-C(6B)-C(7B)	121.6(4)
C(1)-C(19)-H(19A)	109.5
C(1)-C(19)-H(19B)	109.5
C(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(15)-C(16)-C(17)	120.1(5)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
O(1B)-C(11B)-C(1B)	106.8(3)
O(1B)-C(11B)-C(12B)	111.1(4)
O(1B)-C(11B)-H(11B)	107.7
C(1B)-C(11B)-H(11B)	107.7
C(12B)-C(11B)-C(1B)	115.5(4)

C(12B)-C(11B)-H(11B)	107.7
C(3)-C(4)-H(4)	119.2
C(5)-C(4)-C(3)	121.5(4)
C(5)-C(4)-H(4)	119.2
C(6)-C(5)-C(4)	119.0(5)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(8B)-C(3B)-C(2B)	123.3(4)
C(8B)-C(3B)-C(4B)	117.5(4)
C(4B)-C(3B)-C(2B)	119.2(4)
C(2B)-C(9B)-H(9B)	118.5
C(10B)-C(9B)-C(2B)	123.0(5)
C(10B)-C(9B)-H(9B)	118.5
C(6)-C(7)-H(7)	120.4
C(8)-C(7)-C(6)	119.2(4)
C(8)-C(7)-H(7)	120.4
C(12B)-C(13B)-H(13B)	119.8
C(14B)-C(13B)-C(12B)	120.4(5)
C(14B)-C(13B)-H(13B)	119.8
C(13B)-C(14B)-H(14B)	120.1
C(13B)-C(14B)-C(15B)	119.8(5)
C(15B)-C(14B)-H(14B)	120.1
C(3B)-C(4B)-H(4B)	119.0
C(5B)-C(4B)-C(3B)	122.0(4)
C(5B)-C(4B)-H(4B)	119.0
C(9B)-C(10B)-H(10C)	120.0
C(9B)-C(10B)-H(10D)	120.0
H(10C)-C(10B)-H(10D)	120.0
C(9)-C(10)-H(10A)	120.0
C(9)-C(10)-H(10B)	120.0
H(10A)-C(10)-H(10B)	120.0
C(14B)-C(15B)-H(15B)	119.9
C(16B)-C(15B)-C(14B)	120.2(5)
C(16B)-C(15B)-H(15B)	119.9
C(12B)-C(17B)-H(17B)	119.6
C(12B)-C(17B)-C(16B)	120.8(5)
C(16B)-C(17B)-H(17B)	119.6
C(6B)-C(5B)-C(4B)	118.9(5)
C(6B)-C(5B)-H(5B)	120.6
C(4B)-C(5B)-H(5B)	120.6
C(15B)-C(16B)-C(17B)	120.1(5)
C(15B)-C(16B)-H(16B)	120.0
C(17B)-C(16B)-H(16B)	120.0

Symmetry transformations used to generate equivalent atoms:

Table A7.4. *Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **117**. The anisotropic displacement factor exponent takes the form*
$-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Br(1)	216(2)	209(2)	285(2)	-37(2)	36(2)	57(2)
Br(1B)	176(2)	307(3)	382(3)	10(2)	76(2)	-18(2)
O(1)	164(16)	123(16)	218(17)	-4(14)	-13(13)	-28(13)
O(1B)	158(17)	130(16)	254(17)	27(13)	-4(14)	-4(13)
O(2B)	144(17)	223(19)	340(20)	29(15)	19(15)	75(15)
O(2)	149(16)	138(18)	430(20)	-13(16)	45(15)	28(13)
C(12)	160(20)	120(20)	190(20)	-7(17)	17(18)	-13(19)
C(18)	140(20)	120(20)	260(20)	-3(18)	8(18)	-9(17)
C(9)	240(20)	120(20)	200(20)	-3(17)	-10(20)	0(20)
C(18B)	160(20)	150(20)	260(20)	20(20)	33(18)	-3(19)
C(8B)	200(20)	110(20)	190(20)	-5(17)	5(19)	-20(20)
C(2B)	131(19)	120(20)	200(20)	15(18)	-1(18)	20(20)
C(1B)	150(20)	110(20)	220(20)	21(19)	-13(17)	0(18)
C(1)	150(20)	120(20)	190(20)	-8(17)	0(17)	8(17)
C(15)	360(30)	220(30)	130(20)	13(19)	-30(20)	-30(20)
C(14)	270(30)	200(20)	170(20)	11(18)	60(19)	-20(20)
C(11)	120(20)	130(20)	210(20)	20(18)	20(17)	-36(17)
C(6)	170(20)	190(20)	180(20)	10(18)	-5(18)	56(18)
C(17)	180(20)	240(30)	210(20)	10(20)	16(19)	10(20)
C(2)	140(20)	140(20)	200(20)	10(18)	6(17)	13(18)
C(7B)	180(20)	150(20)	210(20)	-17(18)	11(19)	20(20)
C(8)	150(20)	190(20)	250(20)	-13(19)	-1(19)	-20(19)
C(3)	140(20)	150(20)	136(19)	-1(16)	-2(17)	15(19)
C(13)	140(20)	190(20)	200(20)	5(19)	37(18)	-7(19)
C(19B)	200(20)	140(20)	230(20)	-3(18)	40(20)	10(20)
C(12B)	180(20)	140(20)	220(20)	5(18)	-18(18)	-6(18)
C(6B)	170(20)	250(30)	200(20)	-10(20)	3(18)	0(20)
C(19)	170(20)	240(30)	200(20)	0(20)	-18(17)	-60(20)
C(16)	200(20)	230(30)	240(30)	30(20)	-33(19)	10(20)
C(11B)	150(20)	130(20)	170(20)	20(17)	-14(17)	10(18)
C(4)	150(20)	160(20)	180(20)	0(18)	-5(17)	-22(18)
C(5)	210(20)	140(20)	210(20)	21(18)	0(17)	0(20)
C(3B)	150(20)	140(20)	160(20)	-4(18)	-8(16)	-5(18)
C(9B)	190(20)	190(20)	240(20)	-40(20)	31(19)	-40(20)
C(7)	150(20)	220(20)	200(20)	0(20)	13(19)	3(19)
C(13B)	230(30)	170(20)	240(30)	-20(20)	0(20)	20(20)
C(14B)	260(30)	220(30)	260(30)	-50(20)	40(20)	40(20)
C(4B)	210(30)	140(20)	180(20)	2(17)	0(18)	10(19)
C(10B)	210(30)	260(30)	330(30)	-50(20)	-10(20)	-20(20)
C(10)	330(30)	200(30)	280(30)	40(20)	-30(20)	20(30)
C(15B)	310(30)	330(30)	220(20)	-50(20)	20(20)	-10(30)
C(17B)	190(20)	200(30)	270(20)	-9(19)	-20(20)	40(20)
C(5B)	230(30)	160(30)	240(20)	0(19)	30(20)	-50(20)
C(16B)	280(30)	310(30)	230(20)	10(20)	-30(20)	40(20)

Table A7.5. *Hydrogen coordinates (x 10^3) and isotropic displacement parameters (Å^{2}x 10^3) for* ***117.***

	x	y	z	U_{iso}

H(1)	239	225	480	25
H(1B)	849	462	533	27
H(2B)	1057	523	535	36
H(2)	175	351	533	36
H(18A)	304	472	563	21
H(18B)	273	523	498	21
H(9)	364	515	380	22
H(18C)	963	619	469	23
H(18D)	991	682	530	23
H(8B)	645	792	600	20
H(2BA)	830	574	611	18
H(15)	516	283	748	28
H(14)	327	319	728	26
H(11)	422	240	496	19
H(17)	572	250	566	25
H(2A)	244	338	422	19
H(7B)	455	791	632	22
H(8)	518	399	356	24
H(13)	260	320	628	21
H(19D)	838	796	514	29
H(19E)	712	757	502	29
H(19F)	808	740	451	29
H(19A)	476	502	467	30
H(19B)	533	392	471	30
H(19C)	499	451	533	30
H(16)	639	251	667	27
H(11B)	670	570	502	18
H(4)	292	176	394	20
H(5)	398	62	336	23
H(9B)	837	789	628	25
H(7)	622	286	297	23
H(13B)	905	453	425	26
H(14B)	923	439	318	30
H(4B)	666	491	635	21
H(10C)	990	637	660	32
H(10D)	998	757	679	32
H(10A)	140	454	366	32
H(10B)	197	560	341	32
H(15B)	794	521	254	34
H(17B)	630	632	402	26
H(5B)	479	489	666	25
H(16B)	649	618	295	33

Table A7.6. *Hydrogen bonds for* ***117*** *[Å and °].*

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1B)-H(1B)...O(2B)	0.84	1.91	2.669(5)	150.6
O(2B)-H(2B)...O(2)#1	0.84	1.99	2.689(5)	140.2

O(2)-H(2)...O(1)	0.84	1.91	2.629(5)	142.7

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z

***Table A7.7**. Torsion angles [°] for **117**.*

Br(1)-C(6)-C(5)-C(4)	-179.3(3)
Br(1)-C(6)-C(7)-C(8)	179.6(3)
Br(1B)-C(6B)-C(5B)-C(4B)	-178.6(3)
O(2B)-C(18B)-C(1B)-C(2B)	55.2(5)
O(2B)-C(18B)-C(1B)-C(19B)	176.0(4)
O(2B)-C(18B)-C(1B)-C(11B)	-64.4(5)
O(2)-C(18)-C(1)-C(11)	-57.0(5)
O(2)-C(18)-C(1)-C(2)	61.9(5)
O(2)-C(18)-C(1)-C(19)	-176.9(4)
C(12)-C(17)-C(16)-C(15)	0.5(8)
C(18)-C(1)-C(11)-O(1)	63.0(5)
C(18)-C(1)-C(11)-C(12)	-62.6(5)
C(18)-C(1)-C(2)-C(9)	54.6(5)
C(18)-C(1)-C(2)-C(3)	-178.1(4)
C(9)-C(2)-C(3)-C(8)	45.4(6)
C(9)-C(2)-C(3)-C(4)	-132.4(4)
C(18B)-C(1B)-C(11B)-O(1B)	64.1(5)
C(18B)-C(1B)-C(11B)-C(12B)	-60.1(5)
C(8B)-C(7B)-C(6B)-Br(1B)	178.6(3)
C(8B)-C(7B)-C(6B)-C(5B)	0.0(7)
C(8B)-C(3B)-C(4B)-C(5B)	0.6(7)
C(2B)-C(1B)-C(11B)-O(1B)	-54.8(5)
C(2B)-C(1B)-C(11B)-C(12B)	-179.0(4)
C(2B)-C(3B)-C(4B)-C(5B)	177.8(4)
C(1B)-C(2B)-C(3B)-C(8B)	-79.4(5)
C(1B)-C(2B)-C(3B)-C(4B)	103.6(5)
C(1B)-C(2B)-C(9B)-C(10B)	-100.3(5)
C(1)-C(2)-C(3)-C(8)	-83.0(5)
C(1)-C(2)-C(3)-C(4)	99.3(5)
C(15)-C(14)-C(13)-C(12)	0.1(7)
C(14)-C(15)-C(16)-C(17)	-1.0(8)
C(11)-C(12)-C(17)-C(16)	-178.5(4)
C(11)-C(12)-C(13)-C(14)	178.2(4)
C(11)-C(1)-C(2)-C(9)	175.3(4)
C(11)-C(1)-C(2)-C(3)	-57.4(5)
C(17)-C(12)-C(11)-O(1)	137.1(4)
C(17)-C(12)-C(11)-C(1)	-97.0(5)
C(17)-C(12)-C(13)-C(14)	-0.6(7)
C(2)-C(1)-C(11)-O(1)	-56.4(5)
C(2)-C(1)-C(11)-C(12)	178.1(4)
C(2)-C(3)-C(4)-C(5)	178.2(4)
C(7B)-C(8B)-C(3B)-C(2B)	-177.6(4)
C(7B)-C(8B)-C(3B)-C(4B)	-0.6(6)
C(7B)-C(6B)-C(5B)-C(4B)	0.0(7)
C(8)-C(3)-C(4)-C(5)	0.3(7)
C(3)-C(8)-C(7)-C(6)	-0.2(7)
C(3)-C(4)-C(5)-C(6)	-0.6(7)
C(13)-C(12)-C(11)-O(1)	-41.8(6)
C(13)-C(12)-C(11)-C(1)	84.2(5)
C(13)-C(12)-C(17)-C(16)	0.3(7)

C(19B)-C(1B)-C(11B)-O(1B)	-177.8(3)
C(19B)-C(1B)-C(11B)-C(12B)	58.0(5)
C(12B)-C(13B)-C(14B)-C(15B)	-0.1(8)
C(12B)-C(17B)-C(16B)-C(15B)	1.0(8)
C(19)-C(1)-C(11)-O(1)	-177.7(4)
C(19)-C(1)-C(11)-C(12)	56.8(5)
C(19)-C(1)-C(2)-C(9)	-64.8(5)
C(19)-C(1)-C(2)-C(3)	62.5(5)
C(16)-C(15)-C(14)-C(13)	0.7(8)
C(11B)-C(12B)-C(13B)-C(14B)	179.6(5)
C(11B)-C(12B)-C(17B)-C(16B)	180.0(5)
C(5)-C(6)-C(7)-C(8)	0.0(7)
C(3B)-C(8B)-C(7B)-C(6B)	0.3(7)
C(3B)-C(2B)-C(1B)-C(18B)	-172.3(4)
C(3B)-C(2B)-C(1B)-C(19B)	69.9(5)
C(3B)-C(2B)-C(1B)-C(11B)	-51.7(5)
C(3B)-C(2B)-C(9B)-C(10B)	130.2(5)
C(3B)-C(4B)-C(5B)-C(6B)	-0.3(7)
C(9B)-C(2B)-C(1B)-C(18B)	60.0(5)
C(9B)-C(2B)-C(1B)-C(19B)	-57.8(5)
C(9B)-C(2B)-C(1B)-C(11B)	-179.4(4)
C(9B)-C(2B)-C(3B)-C(8B)	49.2(6)
C(9B)-C(2B)-C(3B)-C(4B)	-127.9(4)
C(7)-C(6)-C(5)-C(4)	0.4(7)
C(7)-C(8)-C(3)-C(2)	-177.7(4)
C(7)-C(8)-C(3)-C(4)	0.0(7)
C(13B)-C(12B)-C(11B)-O(1B)	-36.2(6)
C(13B)-C(12B)-C(11B)-C(1B)	85.7(5)
C(13B)-C(12B)-C(17B)-C(16B)	-0.9(7)
C(13B)-C(14B)-C(15B)-C(16B)	0.2(8)
C(14B)-C(15B)-C(16B)-C(17B)	-0.7(8)
C(10)-C(9)-C(2)-C(1)	-120.1(5)
C(10)-C(9)-C(2)-C(3)	110.7(5)
C(17B)-C(12B)-C(11B)-O(1B)	142.9(4)
C(17B)-C(12B)-C(11B)-C(1B)	-95.2(5)
C(17B)-C(12B)-C(13B)-C(14B)	0.5(7)

Symmetry transformations used to generate equivalent atoms: