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

atom	x	y	z	B_{eq}
Br	0.00098(8)	-0.55162(4)	0.0964(2)	4.23(4)
F	-0.2328(5)	-0.4193(3)	0.6212(8)	4.3(1)
O(1)	-0.4254(4)	-0.3503(3)	0.083(1)	3.5(1)
O(2)	-0.2221(5)	-0.1743(3)	0.3024(9)	3.1(1)
O(3)	-0.1607(6)	0.0025(3)	-0.012(1)	4.9(2)
O(4)	-0.1531(4)	-0.2229(3)	-0.231(1)	3.1(1)
N(1)	-0.3710(5)	-0.1879(3)	-0.173(1)	2.1(1)
N(2)	-0.3144(5)	-0.2666(3)	0.184(1)	2.4(1)
N(3)	-0.1351(5)	-0.1083(4)	-0.132(1)	2.9(1)
C(1)	-0.4092(6)	-0.1611(4)	-0.357(1)	2.7(1)
C(2)	-0.4822(6)	-0.2046(4)	-0.428(1)	2.9(1)
C(3)	-0.4876(6)	-0.2612(4)	-0.292(1)	2.8(1)
C(4)	-0.4184(6)	-0.2510(4)	-0.133(1)	2.5(1)
C(5)	-0.3907(6)	-0.2934(4)	0.045(1)	2.4(1)
C(6)	-0.2751(5)	-0.2012(4)	0.167(1)	2.2(1)
C(7)	-0.2898(5)	-0.1611(4)	-0.043(1)	2.0(1)
C(8)	-0.2950(7)	-0.0826(4)	-0.003(2)	2.8(1)
C(9)	-0.1928(7)	-0.0557(4)	-0.046(1)	3.0(2)
C(10)	-0.1846(6)	-0.1698(4)	-0.152(1)	2.3(1)
C(11)	-0.2814(7)	-0.3103(5)	0.362(1)	2.9(2)
C(12)	-0.2114(6)	-0.3670(4)	0.288(1)	2.4(1)
C(13)	-0.1886(7)	-0.4212(4)	0.423(1)	2.7(1)
C(14)	-0.1260(6)	-0.4766(4)	0.373(2)	3.0(2)
C(15)	-0.0819(6)	-0.4757(4)	0.178(2)	2.7(1)

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

atom	x	y	z	B_{eq}
C(16)	-0.1007(8)	-0.4241(5)	0.035(2)	3.4(2)
C(17)	-0.1647(6)	-0.3698(5)	0.089(1)	2.9(1)
H(1)	-0.3891	-0.1191	-0.4246	3.0927
H(2)	-0.5214	-0.1981	-0.5543	3.6439
H(3)	-0.5319	-0.3002	-0.3055	3.3636
H(4)	-0.3426	-0.0618	-0.0980	3.5760
H(5)	-0.3141	-0.0727	0.1392	3.5760
H(6)	-0.2479	-0.2821	0.4636	3.5831
H(7)	-0.3397	-0.3307	0.4242	3.5831
H(8)	-0.0656	-0.1027	-0.1702	3.5752
H(9)	-0.1123	-0.5138	0.4716	3.5570
H(10)	-0.0686	-0.4248	-0.1033	3.9660
H(11)	-0.1773	-0.3325	-0.0104	3.6683

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

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Br	C(15)	1.896(8)	F	C(13)	1.37(1)
O(1)	C(5)	1.212(9)	O(2)	C(6)	1.22(1)
O(3)	C(9)	1.22(1)	O(4)	C(10)	1.211(10)
N(1)	C(1)	1.36(1)	N(1)	C(4)	1.390(9)
N(1)	C(7)	1.442(10)	N(2)	C(5)	1.43(1)
N(2)	C(6)	1.366(10)	N(2)	C(11)	1.46(1)
N(3)	C(9)	1.38(1)	N(3)	C(10)	1.36(1)
C(1)	C(2)	1.35(1)	C(2)	C(3)	1.39(1)
C(3)	C(4)	1.37(1)	C(4)	C(5)	1.43(1)
C(6)	C(7)	1.54(1)	C(7)	C(8)	1.53(1)
C(7)	C(10)	1.56(1)	C(8)	C(9)	1.47(1)
C(11)	C(12)	1.50(1)	C(12)	C(13)	1.38(1)
C(12)	C(17)	1.39(1)	C(13)	C(14)	1.39(1)
C(14)	C(15)	1.36(1)	C(15)	C(16)	1.36(1)
C(16)	C(17)	1.39(1)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
N(3)	H(8)	0.95	C(1)	H(1)	0.95
C(2)	H(2)	0.95	C(3)	H(3)	0.96
C(8)	H(4)	0.96	C(8)	H(5)	0.94
C(11)	H(6)	0.95	C(11)	H(7)	0.95
C(14)	H(9)	0.96	C(16)	H(10)	0.97
C(17)	H(11)	0.97			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	N(1)	C(4)	108.5(6)	C(1)	N(1)	C(7)	128.3(6)
C(4)	N(1)	C(7)	123.1(6)	C(5)	N(2)	C(6)	123.7(7)
C(5)	N(2)	C(11)	117.8(6)	C(6)	N(2)	C(11)	118.4(7)
C(9)	N(3)	C(10)	114.2(7)	N(1)	C(1)	C(2)	108.2(7)
C(1)	C(2)	C(3)	108.5(8)	C(2)	C(3)	C(4)	107.7(7)
N(1)	C(4)	C(3)	107.1(7)	N(1)	C(4)	C(5)	121.6(7)
C(3)	C(4)	C(5)	131.3(7)	O(1)	C(5)	N(2)	118.3(7)
O(1)	C(5)	C(4)	124.9(7)	N(2)	C(5)	C(4)	116.8(6)
O(2)	C(6)	N(2)	123.9(8)	O(2)	C(6)	C(7)	117.3(7)
N(2)	C(6)	C(7)	118.6(7)	N(1)	C(7)	C(6)	113.5(6)
N(1)	C(7)	C(8)	114.4(6)	N(1)	C(7)	C(10)	112.1(6)
C(6)	C(7)	C(8)	111.0(6)	C(6)	C(7)	C(10)	102.0(6)
C(8)	C(7)	C(10)	102.6(6)	C(7)	C(8)	C(9)	105.9(7)
O(3)	C(9)	N(3)	123.6(9)	O(3)	C(9)	C(8)	127.6(8)
N(3)	C(9)	C(8)	108.8(7)	O(4)	C(10)	N(3)	127.4(8)
O(4)	C(10)	C(7)	125.3(7)	N(3)	C(10)	C(7)	107.2(6)
N(2)	C(11)	C(12)	111.4(6)	C(11)	C(12)	C(13)	119.4(7)
C(11)	C(12)	C(17)	125.3(7)	C(13)	C(12)	C(17)	115.3(7)
F	C(13)	C(12)	116.5(7)	F	C(13)	C(14)	118.6(8)
C(12)	C(13)	C(14)	124.9(8)	C(13)	C(14)	C(15)	116.8(8)
Br	C(15)	C(14)	118.9(6)	Br	C(15)	C(16)	119.3(7)
C(14)	C(15)	C(16)	121.7(8)	C(15)	C(16)	C(17)	120.0(8)
C(12)	C(17)	C(16)	121.2(8)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(9)	N(3)	H(8)	123.2	C(10)	N(3)	H(8)	122.5
N(1)	C(1)	H(1)	126.7	C(2)	C(1)	H(1)	125.1
C(1)	C(2)	H(2)	125.5	C(3)	C(2)	H(2)	126.0
C(2)	C(3)	H(3)	126.5	C(4)	C(3)	H(3)	125.8
C(7)	C(8)	H(4)	109.7	C(7)	C(8)	H(5)	111.4
C(9)	C(8)	H(4)	109.9	C(9)	C(8)	H(5)	110.4
H(4)	C(8)	H(5)	109.4	N(2)	C(11)	H(6)	108.9
N(2)	C(11)	H(7)	108.1	C(12)	C(11)	H(6)	109.7
C(12)	C(11)	H(7)	109.1	H(6)	C(11)	H(7)	109.6
C(13)	C(14)	H(9)	122.7	C(15)	C(14)	H(9)	120.5
C(15)	C(16)	H(10)	120.3	C(17)	C(16)	H(10)	119.7
C(12)	C(17)	H(11)	118.3	C(16)	C(17)	H(11)	120.5

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Br	C(15)	C(14)	C(13)	-177.9(6)	Br	C(15)	C(16)	C(17)	177.2(7)
F	C(13)	C(12)	C(11)	0(1)	F	C(13)	C(12)	C(17)	179.4(7)
F	C(13)	C(14)	C(15)	-178.5(7)	O(1)	C(5)	N(2)	C(6)	-174.9(7)
O(1)	C(5)	N(2)	C(11)	1(1)	O(1)	C(5)	C(4)	N(1)	-176.3(7)
O(1)	C(5)	C(4)	C(3)	1(1)	O(2)	C(6)	N(2)	C(5)	168.3(7)
O(2)	C(6)	N(2)	C(11)	-7(1)	O(2)	C(6)	C(7)	N(1)	-166.4(7)
O(2)	C(6)	C(7)	C(8)	-36.0(9)	O(2)	C(6)	C(7)	C(10)	72.8(8)
O(3)	C(9)	N(3)	C(10)	178.2(9)	O(3)	C(9)	C(8)	C(7)	-171.3(9)
O(4)	C(10)	N(3)	C(9)	176.3(8)	O(4)	C(10)	C(7)	N(1)	-48(1)
O(4)	C(10)	C(7)	C(6)	72.9(9)	O(4)	C(10)	C(7)	C(8)	-172.1(8)
N(1)	C(1)	C(2)	C(3)	-2.3(10)	N(1)	C(4)	C(3)	C(2)	0.1(9)
N(1)	C(4)	C(5)	N(2)	1(1)	N(1)	C(7)	C(6)	N(2)	19.2(9)
N(1)	C(7)	C(8)	C(9)	-132.3(7)	N(1)	C(7)	C(10)	N(3)	133.5(7)
N(2)	C(5)	C(4)	C(3)	-179.8(8)	N(2)	C(6)	C(7)	C(8)	149.6(7)
N(2)	C(6)	C(7)	C(10)	-101.6(7)	N(2)	C(11)	C(12)	C(13)	-167.2(7)
N(2)	C(11)	C(12)	C(17)	13(1)	N(3)	C(9)	C(8)	C(7)	7.8(9)
N(3)	C(10)	C(7)	C(6)	-104.7(7)	N(3)	C(10)	C(7)	C(8)	10.3(8)
C(1)	N(1)	C(4)	C(3)	-1.5(9)	C(1)	N(1)	C(4)	C(5)	177.0(7)
C(1)	N(1)	C(7)	C(6)	173.8(7)	C(1)	N(1)	C(7)	C(8)	45(1)
C(1)	N(1)	C(7)	C(10)	-71.2(9)	C(1)	C(2)	C(3)	C(4)	1.4(10)
C(2)	C(1)	N(1)	C(4)	2.4(9)	C(2)	C(1)	N(1)	C(7)	177.7(7)
C(2)	C(3)	C(4)	C(5)	-178.3(8)	C(3)	C(4)	N(1)	C(7)	-177.1(7)
C(4)	N(1)	C(7)	C(6)	-11.6(10)	C(4)	N(1)	C(7)	C(8)	-140.2(7)
C(4)	N(1)	C(7)	C(10)	103.4(8)	C(4)	C(5)	N(2)	C(6)	6(1)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(4)	C(5)	N(2)	C(11)	-177.2(7)	C(5)	N(2)	C(6)	C(7)	-17(1)
C(5)	N(2)	C(11)	C(12)	76.9(9)	C(5)	C(4)	N(1)	C(7)	1(1)
C(6)	N(2)	C(11)	C(12)	-106.9(8)	C(6)	C(7)	C(8)	C(9)	97.7(8)
C(7)	C(6)	N(2)	C(11)	166.3(7)	C(7)	C(10)	N(3)	C(9)	-6.2(9)
C(8)	C(9)	N(3)	C(10)	0(1)	C(9)	C(8)	C(7)	C(10)	-10.6(8)
C(11)	C(12)	C(13)	C(14)	179.5(8)	C(11)	C(12)	C(17)	C(16)	179.6(8)
C(12)	C(13)	C(14)	C(15)	1(1)	C(12)	C(17)	C(16)	C(15)	0(1)
C(13)	C(12)	C(17)	C(16)	0(1)	C(13)	C(14)	C(15)	C(16)	-1(1)
C(14)	C(13)	C(12)	C(17)	-1(1)	C(14)	C(15)	C(16)	C(17)	1(1)

Table 8. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC
Br	O(3)	3.513(8)	54504
Br	F	3.590(6)	44402
F	C(14)	3.16(1)	44502
F	C(17)	3.217(10)	55601
O(1)	O(4)	3.448(8)	44503
O(2)	O(4)	3.207(9)	55601
O(2)	C(3)	3.336(10)	54503
O(3)	C(1)	3.34(1)	45502
O(3)	C(8)	3.60(1)	45502
O(4)	C(11)	3.50(1)	55401
C(1)	C(6)	3.56(1)	55401
C(2)	C(17)	3.52(1)	44503
Br	N(3)	3.581(8)	54404
F	C(16)	3.13(1)	55601
F	C(15)	3.194(10)	44502
O(1)	N(3)	2.898(9)	44503
O(1)	C(10)	3.47(1)	44503
O(2)	C(1)	3.28(1)	55601
O(2)	C(10)	3.46(1)	55601
O(3)	C(8)	3.50(1)	45402
O(4)	C(2)	3.41(1)	54403
N(2)	C(2)	3.50(1)	55601
C(2)	C(12)	3.44(1)	44503
C(2)	C(11)	3.59(1)	55401