

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: 1

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Bond precision:    C-C = 0.0078 A                      Wavelength=0.71073

Cell:              a=6.8486(6)              b=7.3506(7)              c=9.2054(8)  
                    alpha=85.915(1)          beta=79.327(1)          gamma=64.478(1)

Temperature:      298 K

	Calculated	Reported
Volume	410.94(6)	410.94(6)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C10 H10 N2, Br4 O2 U	?
Sum formula	C10 H10 Br4 N2 O2 U	C10 H10 Br4 N2 O2 U
Mr	747.83	747.87
Dx,g cm-3	3.022	3.022
Z	1	1
Mu (mm-1)	19.595	19.595
F000	332.0	332.0
F000'	321.74	
h,k,lmax	9,10,13	9,10,12
Nref	2472	2285
Tmin,Tmax	0.166,0.309	0.166,0.309
Tmin'	0.087	

Correction method= EMPIRICAL

Data completeness= 0.924                      Theta(max)= 30.330

R(reflections)= 0.0255( 2066)              wR2(reflections)= 0.0543( 2285)

S = 1.050                                      Npar= 88

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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.

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### Alert level C

PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C1
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C2
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C3
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	U1
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....		3.28
PLAT432_ALERT_2_C	Short Inter X...Y Contact	O1 .. C5 ..	2.99 Ang.



S = 1.041

Npar= 97

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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.

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● **Alert level C**

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PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) U1 -- Br1 .. 6.76 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) U1 -- Br2 .. 6.51 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for U1
PLAT432_ALERT_2_C Short Inter X...Y Contact O1 .. C5 .. 2.99 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1 .. BR2 .. 2.94 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
C12 H14 N2
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● **Alert level G**

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PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 1000) 400 Deg.
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0 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

6 **ALERT level C** = Check and explain

1 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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## Datablock: 3

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Bond precision: C-C = 0.0052 A

Wavelength=0.71073

Cell: a=7.0925(6)

b=8.4033(9)

c=8.7823(8)

alpha=80.634(2)

beta=73.087(1)

gamma=65.055(1)

Temperature: 298 K

	Calculated	Reported
Volume	453.59(7)	453.59(7)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C12 H12 N2, Br4 O2 U	?
Sum formula	C12 H12 Br4 N2 O2 U	C12 H12 Br4 N2 O2 U
Mr	773.87	773.91
Dx,g cm-3	2.833	2.833
Z	1	1
Mu (mm-1)	17.758	17.758
F000	346.0	346.0
F000'	335.73	
h,k,lmax	10,11,12	10,11,12
Nref	2709	2496
Tmin,Tmax	0.290,0.587	0.447,0.712
Tmin'	0.163	

Correction method= EMPIRICAL

Data completeness= 0.921

Theta(max)= 30.260

R(reflections)= 0.0189( 2397)

wR2(reflections)= 0.0464( 2496)

S = 1.004

Npar= 97

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 C

PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) U1 -- Br1 .. 6.46 su  
 PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for U1

0 ALERT level A = In general: serious problem

0 ALERT level B = Potentially serious problem

2 ALERT level C = Check and explain

0 ALERT level G = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

0 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

## Datablock: 4

Bond precision: C-C = 0.0065 A

Wavelength=0.71073

Cell: a=8.1574(4) b=9.8222(4) c=9.8893(4)  
 alpha=94.769(1) beta=100.771(1) gamma=91.591(1)  
 Temperature: 298 K

	Calculated	Reported
Volume	774.95(6)	774.95(6)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C10 H11 N3), Br4 O2 U, 2(Br), 2(O)	?
Sum formula	C20 H22 Br6 N6 O4 U	C20 H26 BR6 N6 O4 U
Mr	1127.87	1131.96
Dx,g cm-3	2.417	2.426
Z	1	1
Mu (mm-1)	13.006	13.006
F000	518.0	522.0
F000'	507.20	
h,k,lmax	11,13,14	11,13,13
Nref	4691	4295
Tmin,Tmax	0.463,0.771	0.463,0.771
Tmin'	0.350	

Correction method= EMPIRICAL

Data completeness= 0.916

Theta(max)= 30.420

R(reflections)= 0.0331( 3394)

wR2(reflections)= 0.0740( 4295)

S = 1.001

Npar= 173

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 A

PLAT306\_ALERT\_2\_A Isolated Oxygen Atom (H-atoms Missing ?) ..... OW1

#### Alert level C

PLAT222\_ALERT\_3\_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.50 Ratio  
 PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for U1  
 PLAT245\_ALERT\_2\_C U(iso) HN2 Smaller than U(eq) N2 by ... 0.01 AngSq  
 PLAT352\_ALERT\_3\_C Short N-H Bond (0.87A) N2 - HN2 ... 0.73 Ang.  
 PLAT431\_ALERT\_2\_C Short Inter HL..A Contact Br3 .. OW1 .. 3.26 Ang.  
 PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ ?  
 PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... ?  
 PLAT153\_ALERT\_1\_C The su's on the Cell Axes are Equal (x 100000) 40 Ang.  
 PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H1 .. BR3 .. 3.06 Ang.

#### Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
 Atom count from \_chemical\_formula\_sum: C20 H26 Br6 N6 O4 U1  
 Atom count from the \_atom\_site data: C20 H22 Br6 N6 O4 U1

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
 From the CIF: \_cell\_formula\_units\_Z 1  
 From the CIF: \_chemical\_formula\_sum C20 H26 Br6 N6 O4 U  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	20.00	20.00	0.00
H	26.00	22.00	4.00
Br	6.00	6.00	0.00
N	6.00	6.00	0.00
O	4.00	4.00	0.00
U	1.00	1.00	0.00

PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal (x 10000) 100 Deg.  
 PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2

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- 1 **ALERT level A** = In general: serious problem  
 0 **ALERT level B** = Potentially serious problem  
 9 **ALERT level C** = Check and explain  
 5 **ALERT level G** = General alerts; check
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 5 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  
 2 ALERT type 4 Improvement, methodology, query or suggestion  
 0 ALERT type 5 Informative message, check
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## Datablock: 5

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**Bond precision:** C-C = 0.0131 A                      **Wavelength=0.71073**

**Cell:**                      **a=8.6949(10)**                      **b=9.0059(11)**                      **c=11.7255(14)**  
                                  **alpha=79.156(2)**                      **beta=74.365(2)**                      **gamma=82.360(2)**

**Temperature:**    298 K

	Calculated	Reported
Volume	865.12(18)	865.12(18)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C13 H16 N2), Br4 O2 U, 2(Br)	?
Sum formula	C26 H32 Br6 N4 O2 U	C26 H32 Br6 N4 O2 U
Mr	1149.99	1150.05
Dx,g cm-3	2.207	2.207
Z	1	1
Mu (mm-1)	11.647	11.647
F000	534.0	534.0
F000'	523.17	
h,k,lmax	12,12,16	12,12,16
Nref	5104	4628
Tmin,Tmax	0.577,0.792	0.463,0.771
Tmin'	0.390	

Correction method= EMPIRICAL

Data completeness= 0.907

Theta(max)= 30.120

R(reflections)= 0.0473( 2960)

wR2(reflections)= 0.1163( 4628)

S = 1.030

Npar= 178

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 C

PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	C6
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C5
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds (x 1000) Ang ..	13
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C5 -- C6 ..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C7 -- C8 ..	0.19 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		U1
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1
	C13 H16 N2		
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		3
	Br		

### Alert level G

PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal (x 10000)	200 Deg.
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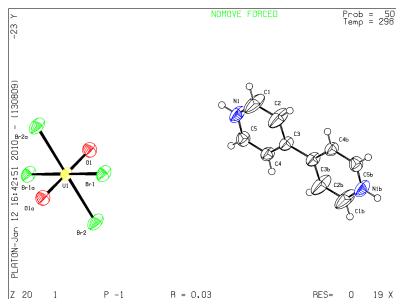
- 0 ALERT level A = In general: serious problem
- 0 ALERT level B = Potentially serious problem
- 8 ALERT level C = Check and explain
- 1 ALERT level G = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 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

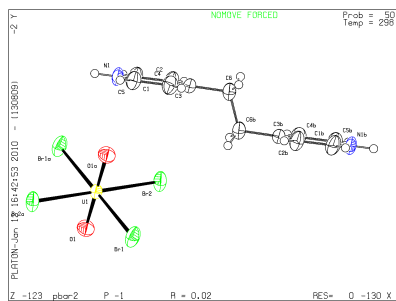
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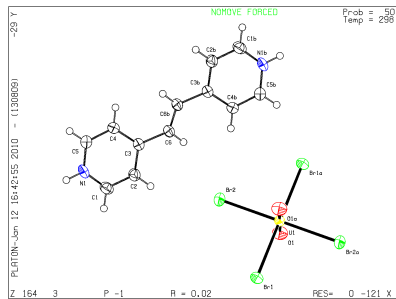
Database 1 - refined plot



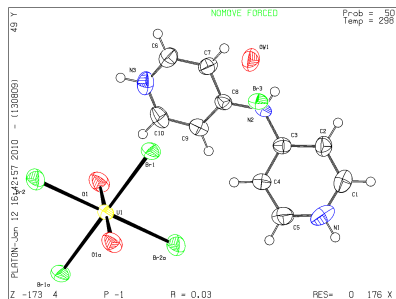
Database plot2 - refined plot



Database 3 - refined plot



Database 4 - refined plot



Database 5 - refined plot

