checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2, 3, 4, 5, 6, 7Th, 7U, 8

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 2

```
Bond precision:   C-C = 0.0068 A              Wavelength=0.71073

Cell:          a=10.0013(4)       b=12.7959(4)       c=15.2146(6)
               alpha=70.674(3)    beta=82.397(3)    gamma=75.020(3)
Temperature:   150 K

                 Calculated                   Reported
Volume           1772.60(12)                  1772.61(12)
Space group      P -1                         P -1
Hall group       -P 1                         -P 1
Moiety formula   C48 H120 I2 N4 Si8 U2        C48 H120 I2 N4 Si8 U2
Sum formula      C48 H120 I2 N4 Si8 U2        C48 H120 I2 N4 Si8 U2
Mr               1708.06                      1708.05
Dx,g cm-3        1.600                        1.600
Z                1                            1
Mu (mm-1)        5.599                        5.599
F000             838.0                        838.0
F000'            818.73
h,k,lmax         12,15,18                     12,15,18
Nref             6480                         6475
Tmin,Tmax        0.689,0.817                  0.844,1.000
Tmin'            0.605

Correction method= # Reported T Limits: Tmin=0.844 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.999         Theta(max)= 25.349

R(reflections)= 0.0307( 5552)     wR2(reflections)= 0.0507( 6475)

S = 1.002                   Npar= 309
```

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   2 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H2A   -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C   -0.31 eA-3

Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1   --I1   .   6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1   --I1_a   .   14.5 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   1 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 3

Bond precision: C-C = 0.0062 A   Wavelength=0.71073

Cell: a=9.6931(3)   b=12.7104(4)   c=15.0496(4)
               alpha=71.469(3)   beta=85.298(2)   gamma=78.226(3)
Temperature: 150 K

	Calculated	Reported
Volume	1720.74(10)	1720.75(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H120 I2 N4 Si8 U2	C48 H120 I2 N4 Si8 U2
Sum formula	C48 H120 I2 N4 Si8 U2	C48 H120 I2 N4 Si8 U2
Mr	1708.06	1708.05
Dx,g cm-3	1.648	1.648
Z	1	1
Mu (mm-1)	5.768	5.768
F000	838.0	838.0
F000'	818.73	
h,k,lmax	11,15,18	11,15,18
Nref	6311	6305
Tmin,Tmax	0.553,0.808	0.712,0.954
Tmin'	0.498	

```
Correction method= # Reported T Limits: Tmin=0.712 Tmax=0.954
AbsCorr = GAUSSIAN


Data completeness= 0.999          Theta(max)= 25.350


R(reflections)= 0.0253( 5549)     wR2(reflections)= 0.0480( 6305)


S = 1.014                Npar= 307
```

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

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       3.3 Ratio
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        C4 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H5A              -0.50 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

⚪ Alert level G

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1        --I1       .     11.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1        --I1_a     .     11.0 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        4 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 4

```
Bond precision:  C-C = 0.0073 A        Wavelength=0.71073

Cell:          a=10.8290(5)    b=12.4282(5)      c=12.9502(5)
               alpha=90        beta=94.783(4)    gamma=90
Temperature:   150 K
```

```
                 Calculated              Reported
Volume           1736.83(13)             1736.85(13)
Space group      P 2/n                   P 1 2/n 1
Hall group       -P 2yac                 -P 2yac
Moiety formula   C26 H58 I2 N O2 Si2 U   C26 H58 I2 N O2 Si2 U
Sum formula      C26 H58 I2 N O2 Si2 U   C26 H58 I2 N O2 Si2 U
Mr               964.74                  964.74
Dx,g cm-3        1.845                   1.845
Z                2                       2
Mu (mm-1)        6.541                   6.541
F000             926.0                   926.0
F000'            905.58
h,k,lmax         13,14,15                13,14,15
Nref             3183                    3182
Tmin,Tmax        0.732,0.780             0.876,0.962
Tmin'            0.639
```

Correction method= # Reported T Limits: Tmin=0.876 Tmax=0.962
AbsCorr = GAUSSIAN

Data completeness= 1.000   Theta(max)= 25.348

R(reflections)= 0.0319(2654)   wR2(reflections)= 0.0518(3182)

S = 1.004   Npar= 171

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
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

---

⚪ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records   1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   1 Report
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   6% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   67 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note

---

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   8 **ALERT level G** = General information/check it is not something unexpected

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

```
    3 ALERT type 2 Indicator that the structure model may be wrong or deficient
    3 ALERT type 3 Indicator that the structure quality may be low
    3 ALERT type 4 Improvement, methodology, query or suggestion
    0 ALERT type 5 Informative message, check
```

Datablock: 5

Bond precision: C-C = 0.0300 A   Wavelength=0.71073

Cell:	a=18.5833(3)	b=18.5833(3)	c=27.7469(8)
	alpha=90	beta=90	gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	9582.1(4)	9582.1(5)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C36 H84 I N2 Si4 U [+ solvent]	C36 H84 I N2 Si4 U
Sum formula	C36 H84 I N2 Si4 U [+ solvent]	C36 H84 I N2 Si4 U
Mr	1022.34	1022.34
Dx,g cm-3	1.417	1.417
Z	8	8
Mu (mm-1)	4.156	4.156
F000	4120.0	4120.0
F000'	4042.90	
h,k,lmax	22,22,33	22,22,33
Nref	4382	4372
Tmin,Tmax	0.593,0.753	0.846,1.000
Tmin'	0.558	

Correction method= # Reported T Limits: Tmin=0.846 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.998   Theta(max)= 25.338

R(reflections)= 0.0880(3542)   wR2(reflections)= 0.2119(4372)

S = 1.154   Npar= 320

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
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.03 Ang.

Author Response: Low C-C bond precision is the result of unresolved modulation in the diffraction data which presents as two versions of the entire molecule, pointing in opposite directions along the U-I axis. Typically this can be resolved to some degree by modelling the entire structure over two positions and refining them competetively with strong restraints on the second (low occupancy) component; however in this instance the large amount of disorder about Si2 made modelling the modulation in this way unsatisfactory and did not result in a better model. This modulation also results in a larger than normal residual peak which we have attributed to the second U component.

🟡 **Alert level C**

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of       U1 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      Si1 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn    H8B      ..H9BB      ..    1.85 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......  11.908 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.584 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).       9 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H13A           -0.31 eA-3
```

⚪ **Alert level G**

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       34 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   922.90 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1        --I1        .    13.1 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      50% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure      127 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        6 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      511 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed         ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 15 ALERT level G = General information/check it is not something unexpected

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

Datablock: 6

```
Bond precision:   C-C = 0.0105 A          Wavelength=0.71073
```

```
Cell:             a=13.7126(5)     b=14.0731(6)       c=20.7186(10)
                  alpha=90         beta=99.150(4)     gamma=90
Temperature:      150 K


                  Calculated                 Reported
Volume            3947.4(3)                  3947.4(3)
Space group       P 21/n                     P 1 21/n 1
Hall group        -P 2yn                     -P 2yn
Moiety formula    C28 H68 I N2 O Si4 U       C28 H68 I N2 O Si4 U
Sum formula       C28 H68 I N2 O Si4 U       C28 H68 I N2 O Si4 U
Mr                926.13                     926.13
Dx,g cm-3         1.558                      1.558
Z                 4                          4
Mu (mm-1)         5.037                      5.037
F000              1836.0                     1836.0
F000'             1797.48
h,k,lmax          16,16,24                   16,16,24
Nref              7222                       7188
Tmin,Tmax         0.658,0.735                0.782,1.000
Tmin'             0.022


Correction method= # Reported T Limits: Tmin=0.782 Tmax=1.000
AbsCorr = GAUSSIAN


Data completeness= 0.995          Theta(max)= 25.347


R(reflections)= 0.0470( 5248)      wR2(reflections)= 0.0701( 7188)


S = 0.987                   Npar= 352
```

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**
```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C8AA Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.01047 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       29 Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on        U2      1.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1AA            -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9              -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16B            -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8AB            -0.42 eA-3
```

⚪ **Alert level G**
```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       37 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....     0.76 mm
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........       32 Note
```

```
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         306 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).           3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600           2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.           1 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

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

Datablock: 7Th

```
Bond precision:   C-C = 0.0170 A          Wavelength=0.71073

Cell:             a=55.079(2)     b=13.3829(7)        c=18.9888(9)
                  alpha=90        beta=95.335(5)      gamma=90
Temperature:      150 K

                  Calculated                Reported
Volume            13936.3(11)               13936.3(11)
Space group       C 2/c                     C 1 2/c 1
Hall group        -C 2yc                    -C 2yc
Moiety formula    C48 H118 Cl2 N4 Si8 Th2   C48 H118 Cl2 N4 Si8 Th2
Sum formula       C48 H118 Cl2 N4 Si8 Th2   C48 H118 Cl2 N4 Si8 Th2
Mr                1511.17                   1511.16
Dx,g cm-3         1.441                     1.440
Z                 8                         8
Mu (mm-1)         4.509                     4.509
F000              6080.0                    6080.0
F000'             5974.00
h,k,lmax          66,16,22                  66,16,22
Nref              12769                     12706
Tmin,Tmax         0.535,0.709               0.937,0.983
Tmin'             0.326

Correction method= # Reported T Limits: Tmin=0.937 Tmax=0.983
AbsCorr = GAUSSIAN

Data completeness= 0.995        Theta(max)= 25.350

R(reflections)= 0.0707( 7130)     wR2(reflections)= 0.1713( 12706)
```

```
S = 1.012                    Npar= 684
```

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
```
PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on      Th1      3.70 eA-3
```

> **Author Response: No chemically sensible species can be assigned to this position. The residual density is located symmetrically either side of the Th atoms and is attributed to imperfect absorption correction. Face indexing of the crystal, combined with a smaller reduction mask as well as a strong absorber correction failed to account for the density. Finally, a larger frame scan range for the background was used, which also did not result in any reduction of the residual density.**

```
PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on      Th2B     2.88 eA-3
```

> **Author Response: No chemically sensible species can be assigned to this position. The residual density is located symmetrically either side of the Th atoms and is attributed to imperfect absorption correction. Face indexing of the crystal, combined with a smaller reduction mask as well as a strong absorber correction failed to account for the density. Finally, a larger frame scan range for the background was used, which also did not result in any reduction of the residual density.**

🟠 Alert level B
```
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).      34 Note
```

> **Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows.**

```
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.06A   From Th1         2.58 eA-3
```

🟡 Alert level C
```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.122
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........   0.122 Report
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range     3.4 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range     4.1 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.01695 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   3.092 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600       23 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....      4 Note
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .    1.39 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03A   From Th1          2.32 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00A   From Th2A         2.08 eA-3
```

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.   0.97A    From Th2B          2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.   1.00A    From Th1           1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.   0.82A    From Th1          -1.89 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.   0.94A    From Th1          -1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.   0.88A    From Th1          -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.   0.83A    From Th1          -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14B            -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18A            -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26A            -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H34B            -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47E            -0.38 eA-3
```

⬤ **Alert level G**
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        43 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        74 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         8 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       16% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1140 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         6 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         8 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
```

```
  2 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
 22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 11 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 21 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 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
```

Datablock: 7U

```
Bond precision:   C-C = 0.0190 A          Wavelength=0.71073

Cell:          a=23.6408(16)    b=10.9612(13)    c=27.4164(15)
               alpha=90         beta=97.384(6)   gamma=90
Temperature:   150 K
```

```
                    Calculated                  Reported
Volume              7045.5(10)                  7045.6(10)
Space group         C 2/c                       C 1 2/c 1
Hall group          -C 2yc                      -C 2yc
Moiety formula      C48 H118 Cl2 N4 Si8 U2      C48 H118 Cl2 N4 Si8 U2
Sum formula         C48 H118 Cl2 N4 Si8 U2      C48 H118 Cl2 N4 Si8 U2
Mr                  1523.14                     1523.14
Dx,g cm-3           1.436                       1.436
Z                   4                           4
Mu (mm-1)           4.834                       4.834
F000                3056.0                      3056.0
F000'               2983.64
h,k,lmax            28,13,33                    28,13,33
Nref                6468                        6459
Tmin,Tmax           0.617,0.695                 0.913,0.981
Tmin'               0.283
```

Correction method= # Reported T Limits: Tmin=0.913 Tmax=0.981
AbsCorr = GAUSSIAN

Data completeness= 0.999   Theta(max)= 25.350

R(reflections)= 0.0609(3184)   wR2(reflections)= 0.1580(6459)

S = 1.006   Npar= 484

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

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..       49% Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.019 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).       10 Note
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.93A    From U1          -1.58 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on        U1    1.50 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.        0 Info
```

⚪ Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       21 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       50 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     7.37 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      56% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       30 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C21B     --C23B        1.74 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       73 Check
            U1   -C1A  -H1AC    1.555    1.555    1.555        35.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      249 Check
```

```
                    U1   -C19B -H19D    1.555   1.555   1.555              28.70 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..............      737 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .         1 Units
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

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

Datablock: 8

```
Bond precision:   C-C = 0.0068 A          Wavelength=0.71073

Cell:           a=21.5207(11)    b=13.1782(5)       c=18.0083(14)
                alpha=90         beta=110.869(8)    gamma=90
Temperature:    150 K

                 Calculated                Reported
Volume           4772.2(5)                 4772.2(5)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C36 H88 N3 Si6 Th         C36 H88 N3 Si6 Th
Sum formula      C36 H88 N3 Si6 Th         C36 H88 N3 Si6 Th
Mr               963.67                    963.67
Dx,g cm-3        1.341                     1.341
Z                4                         4
Mu (mm-1)        3.301                     3.301
F000             1996.0                    1996.0
F000'            1969.54
h,k,lmax         25,15,21                  25,15,21
Nref             4365                      4339
Tmin,Tmax        0.751,0.841               0.935,1.000
Tmin'            0.247

Correction method= # Reported T Limits: Tmin=0.935 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.994          Theta(max)= 25.349

R(reflections)= 0.0395( 3598)     wR2(reflections)= 0.0751( 4339)
```

```
S = 1.110                    Npar= 237
```

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

```
PLAT324_ALERT_2_C Check for Possibly Missing H on Coordinating....      N1 Check
PLAT324_ALERT_2_C Check for Possibly Missing H on Coordinating....      N2 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   3.291 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).       8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600      18 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Info
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      25 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records       1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records       1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Th1      --Si1       .     8.8 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Th1       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1AB      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1AC      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A      Constrained at     0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )       7% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      10 Check
          N1  -SI1 -TH1     1.555   1.555   2.655          39.46 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      20 Check
          C1A -SI1  -C1     1.555   1.555   1.555          14.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      23 Check
          N1  -SI2 -TH1     1.555   1.555   2.655          39.07 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       8 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     212 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       2 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  21 ALERT level G = General information/check it is not something unexpected

   0 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
   6 ALERT type 3 Indicator that the structure quality may be low
  16 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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* or *IUCrData*, 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 13/12/2017; check.def file version of 12/12/2017

NOMOVE FORCED

Prob = 50
Temp = 150

O Y

PLATON-Jan 10 11:27:28 2018 - (70316)

Z 44   5   I 41/a   R = 0.09   RES=   0   0 X