checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_tca_i2_0m

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: cu_tca_i2_0m

```
Bond precision:   C-C = 0.0089 A          Wavelength=1.54178

Cell:              a=20.9574(1)      b=20.9574(1)      c=20.9574(1)
                   alpha=90          beta=90           gamma=90
Temperature:       301 K
```

	Calculated	Reported
Volume	9204.75(13)	9204.75(13)
Space group	I 2 3	I 2 3
Hall group	I 2 2 3	I 2 2 3
Moiety formula	2(C21 H12 N O6), 2(C21 H15 N O6), 2(C H I3), 3(H O), 6(H4 N)	2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 2(C H I3
Sum formula	C86 H83 I6 N10 O27	C86 H83 I6 N10 O27
Mr	2450.02	2450.02
Dx,g cm-3	1.768	1.768
Z	4	4
Mu (mm-1)	16.597	16.597
F000	4812.0	4812.0
F000'	4819.46	
h,k,lmax		23,24,23
Nref		2458
Tmin,Tmax	0.117,0.136	0.559,0.752
Tmin'	0.012	

```
Correction method= # Reported T Limits: Tmin=0.559 Tmax=0.752
AbsCorr = CYLINDER

Data completeness=                 Theta(max)= 62.548
```

R(reflections)= 0.0748(2098)

wR2(reflections)= 0.2104(2458)

S = 1.150 Npar= 190

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

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.500
          From the CIF: _refine_ls_abs_structure_Flack_su   20.000
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5756
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C21 H12 N O6), 2(C21 H15 N O6), 2(C H I3), 3(H O), 6(H4 N)
             Rep.: 2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 2(C H
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.07 Note
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          2 Check
             I1      C4
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.8 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O00M      0.200 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00893 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C21 H12 N O6
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
               0  0  4,
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Report
             H003  H00M  H00B  H00C  H00G  H00H
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.500 Note
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H00M       Constrained at        0.5 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  I1       ..C00J     .       3.48 Ang.
                                    1/2+y,-1/2+z,-1/2+x  =     21_544 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         36 Note
             O001    O002    O003    H003    O004    N005    N006    H00B
             H00C    H00G    H00H    C007    C008    C009    C00A    H00A
             C00B    C00C    C00D    H00D    C00E    H00E    C00F    H00F
             N00G    C00H    C00I    H00I    C00J    H00J    C00K    H00K
             C00L    H00L    O00M    H00M
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        69% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  1  1,   0  0  2,
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
```

```
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
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   3 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
   9 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_STRVA01_cu_tca_i2_0m
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_THETM01_cu_tca_i2_0m
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.590
RESPONSE: ...
;
_vrf_PLAT042_cu_tca_i2_0m
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT090_cu_tca_i2_0m
;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ........       7.07 Note
RESPONSE: ...
;
_vrf_PLAT202_cu_tca_i2_0m
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent .........          2 Check
RESPONSE: ...
;
_vrf_PLAT250_cu_tca_i2_0m
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.5 Note
RESPONSE: ...
;
_vrf_PLAT260_cu_tca_i2_0m
;
PROBLEM: Large Average Ueq of Residue Including      O00M      0.200 Check
RESPONSE: ...
;
_vrf_PLAT342_cu_tca_i2_0m
;
```

```
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00893 Ang.
RESPONSE: ...
;
_vrf_PLAT790_cu_tca_i2_0m
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
RESPONSE: ...
;
_vrf_PLAT918_cu_tca_i2_0m
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
RESPONSE: ...
;
_vrf_PLAT934_cu_tca_i2_0m
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
RESPONSE: ...
;
_vrf_PLAT987_cu_tca_i2_0m
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 14/11/2023; check.def file version of 14/09/2023

Datablock cu_tca_i2_0m - ellipsoid plot