checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1_a

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Bond precision:  C-C = 0.0125 A          Wavelength=1.34139

Cell:            a=14.084(3)     b=21.139(4)         c=25.582(5)
                 alpha=90        beta=104.66(3)      gamma=90
Temperature:     190 K
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	Calculated	Reported
Volume	7368(3)	7368(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C51 H120 K2 N13 P6 U3	C51 H120 K2 N13 P6 U3
Sum formula	C51 H120 K2 N13 P6 U3	C51 H120 K2 N13 P6 U3
Mr	1893.72	1893.70
Dx,g cm-3	1.707	1.707
Z	4	4
Mu (mm-1)	15.509	14.982
F000	3684.0	3684.0
F000’	3651.70	
h,k,lmax	16,25,30	16,25,30
Nref	13520	13485
Tmin,Tmax	0.207,0.224	0.321,0.751
Tmin’	0.133	

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Correction method= # Reported T Limits: Tmin=0.321 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 53.962

R(reflections)= 0.0328( 11830)    wR2(reflections)= 0.0813( 13485)

S = 1.030                 Npar= 714
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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.

Alert level C

```
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       3.52 %
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.8 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C40 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01252 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C22      - C23      .       1.40 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1       --H1       .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N2       --H2       .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3       --H3       .     Please Check
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         13 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      21.72 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          3 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         1% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H44A     ..H42D     .       2.01 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H44C     ..H42D     .       1.31 Ang.
                                             x,y,z  =      1_555 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT793_ALERT_4_G Model has Chirality at P5          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N7          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at N10         (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at N13         (Centro SPGR)          R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for U1        (IV)      .       3.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for U2        (IV)      .       4.01 Info
PLAT794_ALERT_5_G Tentative Bond Valency for U3        (IV)      .       4.00 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         64 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value     0.0137 Check
PLAT984_ALERT_1_G The  K-f'=    0.3891 Deviates from the B&C-Value     0.3778 Check
PLAT984_ALERT_1_G The  N-f'=    0.0253 Deviates from the B&C-Value     0.0241 Check
PLAT984_ALERT_1_G The  P-f'=    0.2596 Deviates from the B&C-Value     0.2543 Check
PLAT984_ALERT_1_G The  U-f'=   -5.2580 Deviates from the B&C-Value    -3.9641 Check
PLAT985_ALERT_1_G The  K-f"=    0.8535 Deviates from the B&C-Value     0.8310 Check
PLAT985_ALERT_1_G The  P-f"=    0.3354 Deviates from the B&C-Value     0.3332 Check
PLAT985_ALERT_1_G The  U-f"=   11.3041 Deviates from the B&C-Value    10.8496 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
8 ALERT type 4 Improvement, methodology, query or suggestion
4 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 18/09/2020; check.def file version of 20/08/2020

Datablock 1_a - ellipsoid plot