checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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 = 0.0134 A          Wavelength=1.34139

Cell:           a=14.0323(3)    b=21.1682(4)        c=25.5817(5)
                alpha=90        beta=104.430(1)     gamma=90
Temperature:    193 K

                Calculated                Reported
Volume          7359.0(3)                 7359.0(3)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  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       1.709                     1.709
Z               4                         4
Mu (mm-1)       15.528                    15.528
F000            3684.0                    3684.0
F000'           3651.70
h,k,lmax        16,25,30                  16,25,30
Nref            13467                     13433
Tmin,Tmax       0.265,0.212               0.418,0.751
Tmin'           0.169

Correction method= # Reported T Limits: Tmin=0.418 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 53.884

R(reflections)= 0.0349( 10333)    wR2(reflections)= 0.0743( 13433)

S = 1.006                 Npar= 729
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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

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference P3       --C31      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C16      --C17      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22      --C23      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31      --C32      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37      --C39      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43      --C44      .       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         P4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
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        C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C40 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C43 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01337 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C37      - C39      .       1.38 Ang.
PLAT390_ALERT_3_C Deviating Methyl C39       X-C-H Bond Angle ....        103 Degree
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H17C     ..H20A     .       1.89 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H29C     ..H32A     .       1.88 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H37A     ..H39C     .       1.88 Ang.
                                                    x,y,z  =      1_555 Check
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
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.158 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         20 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.98A   From N1            -0.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1              -0.47 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3              -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H39B            -0.36 eA-3
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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.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      11.53 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1       --N1       .        5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1'      --N1       .        8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1'      --N2       .        9.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1'      --N5       .        6.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U1'      --N6       .        6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2'      --N3       .        9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2'      --N8       .        5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2'      --N9       .        7.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of U1         Constrained at       0.98 Check
PLAT300_ALERT_4_G Atom Site Occupancy of U2         Constrained at       0.98 Check
PLAT300_ALERT_4_G Atom Site Occupancy of U3         Constrained at       0.98 Check
PLAT300_ALERT_4_G Atom Site Occupancy of U1'        Constrained at       0.02 Check
PLAT300_ALERT_4_G Atom Site Occupancy of U2'        Constrained at       0.02 Check
PLAT300_ALERT_4_G Atom Site Occupancy of U3'        Constrained at       0.02 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          4% Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.25 Ratio
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K1       --U2'       ..       4.24 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K1       --U3'       ..       4.32 Ang.
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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        151 Check
             N12  -P6   -U3'     1.555   1.555   1.555             32.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        601 Check
             K2   -C39  -H39C    1.555   1.555   1.555             20.20 Deg.
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
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         18 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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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
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  35 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  31 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
  20 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 16/07/2020; check.def file version of 12/07/2020

Datablock 1_a - ellipsoid plot