checkCIF/PLATON report

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

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: 1a

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Bond precision:   C-C = 0.0080 A          Wavelength=1.54178

Cell:               a=9.658(12)      b=25.56(4)          c=18.28(3)
                    alpha=90         beta=90.99(6)       gamma=90
Temperature:        100 K
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	Calculated	Reported
Volume	4512(12)	4511(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C46 H52.50 K0.50 O12.50), 3(H2 O)	C46 H52.5 K0.5 O12.5, 1.5(H2 O)
Sum formula	C92 H111 K O28	C46 H55.50 K0.50 O14
Mr	1703.91	851.95
Dx,g cm-3	1.254	1.254
Z	2	4
Mu (mm-1)	1.164	1.164
F000	1812.0	1812.0
F000'	1818.67	
h,k,lmax	11,31,22	11,30,22
Nref	8729	8036
Tmin,Tmax	0.659,0.673	0.430,0.753
Tmin'	0.598	

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Correction method= # Reported T Limits: Tmin=0.430 Tmax=0.753
AbsCorr = NONE

Data completeness= 0.921            Theta(max)= 71.030

R(reflections)= 0.1822( 5071)                    wR2(reflections)=
                                                 0.4048( 8036)
S = 1.496                  Npar= 559
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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 B

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PLAT082_ALERT_2_B High R1 Value ..................................       0.18 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................       0.40 Report
PLAT149_ALERT_3_B s.u. on the   beta    Angle is Too Large .......       0.06 Degree
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O1       --H1C      .     Please Check
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Alert level C

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.967 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.012 Ang.
PLAT148_ALERT_3_C s.u. on the      b    - Axis is (Too) Large ....     0.0400 Ang.
PLAT148_ALERT_3_C s.u. on the      c    - Axis is (Too) Large ....      0.030 Ang.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O00M     --C01L     .        5.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O010     --C01B     .        5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00M     --C01D     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00S     --C01E     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01A     --C01P     .       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01F Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00I Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00M Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00V Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00Y Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      K016      0.114 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1      0.251 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O2      0.168 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C004     -C00G     .       1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C00H     -C00O     .       1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00797 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C011     - C015     .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C017     - C01D     .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01E     - C01F     .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01G     - C01I     .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01H     - C01L     .       1.36 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H00K     ..H01Q     .       1.98 Ang.
                                                     x,y,z  =      1_555 Check
PLAT415_ALERT_2_C Short Inter D-H..H-X       H1C      ..H01T     .       2.00 Ang.
                                          1-x,-1/2+y,1/2-z  =      2_645 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    19.374 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       270 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        18 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      65.50 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H         .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00E      .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00W      .      -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H01Q      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H01T      .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H01Z      .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on Hc        .      -0.45 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         6 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............         5 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0060 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par    0.0040 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0080 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par    0.0040 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0080 Report
PLAT300_ALERT_4_G Atom Site Occupancy of K016       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B        Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )      100% Note
PLAT303_ALERT_2_G Full Occupancy Atom H01G      with # Connections      1.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )    111.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      1.50 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C014 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C01M Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O00Q     .     108.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       103 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        23 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       412 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  4 ALERT level B = A potentially serious problem, consider carefully
 39 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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 37 ALERT type 2 Indicator that the structure model may be wrong or deficient
 19 ALERT type 3 Indicator that the structure quality may be low
 18 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 06/07/2023; check.def file version of 30/06/2023

Datablock 1a - ellipsoid plot