checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dwat16_0m_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: dwat16_0m_a

Bond precision: C-C = 0.0051 A   Wavelength=0.71073

Cell: a=9.2195(6)   b=5.7344(4)   c=32.1204(16)
               alpha=90   beta=93.209(3)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1695.49(18)	1695.49(18)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H3 I N2 O4, C8 H6 N2 S	2(C8 H3 I N2 O4), 2(C8 H6 N2 S)
Sum formula	C16 H9 I N4 O4 S	C32 H18 I2 N8 O8 S2
Mr	480.23	960.46
Dx,g cm-3	1.881	1.881
Z	4	2
Mu (mm-1)	2.043	2.043
F000	936.0	936.0
F000'	934.97	
h,k,lmax	12,7,42	12,7,42
Nref	4250	4232
Tmin,Tmax	0.536,0.849	0.198,0.263
Tmin'	0.526	

Correction method= # Reported T Limits: Tmin=0.198 Tmax=0.263
AbsCorr = MULTI-SCAN

Data completeness= 0.996   Theta(max)= 28.339

R(reflections)= 0.0438(3944)   wR2(reflections)= 0.1040(4232)

S = 1.164   Npar= 242

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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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    3.314 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H16           -0.37 eA-3
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⚪ Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       5 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    2.00 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records       2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records       1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for     S1'        --C15      .    9.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for     C15        --C14      .    7.5 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )     18% Note
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C2       - C3        .    1.44 Ang.
PLAT431_ALERT_2_G Short Inter HL..A Contact  I1       ..N3        .    2.83 Ang.
                                                    x,y,z  =      1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      30 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      17 Note
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.       3 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
   2 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 07/08/2019; check.def file version of 30/07/2019