checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C8OBTBTOC8rtHB

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: C8OBTBTOC8rtHB

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Bond precision:  C-C = 0.0204 A          Wavelength=0.70000

Cell:             a=31.056(6)     b=7.663(2)         c=5.996(1)
                  alpha=90        beta=94.18(3)      gamma=90
Temperature:      298 K

                Calculated                Reported
Volume          1423.2(5)                 1423.1(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C30 H40 O2 S2             C60 H80 O4 S4
Sum formula     C30 H40 O2 S2             C60 H80 O4 S4
Mr              496.74                    993.48
Dx,g cm-3       1.159                     1.159
Z               2                         1
Mu (mm-1)       0.200                     0.200
F000            536.0                     536.0
F000'           536.65
h,k,lmax        25,6,4                    25,6,4
Nref            818                       806
Tmin,Tmax       0.995,0.998               0.475,0.744
Tmin'           0.984

Correction method= # Reported T Limits: Tmin=0.475 Tmax=0.744
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 16.664

R(reflections)= 0.0951( 473)      wR2(reflections)= 0.2835( 806)

S = 1.014                 Npar= 79
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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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4097

Author Response: Crystals diffracted poorly at RT (best ones show reflections at a maximum resolution of ~1.25 Ang). Radiation damage have been found and limited the maximum dose allowed per data collection.

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) ..... 15 Report

Author Response: Crystals diffracted poorly at RT (best ones show reflections at a maximum resolution of ~1.25 Ang), so few data were available for refinement. Number of model parameters have been kept low to avoid overrefinement. Anisotropic thermal motion modelling have been applied only to sulphur and oxygen atoms.

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0204 Ang.

Author Response: Crystals diffracted poorly at RT (best ones show reflections at a maximum resolution of ~1.25 Ang) and were prone to radiation damage. This error is due to high model e.s.d., mainly found on terminal atoms of flexible hydrocarburic tails.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.146

PLAT020_ALERT_3_C The value of Rint is greater than 0.12	0.146	Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.6	Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C20_1	Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...	-0.187	Report
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.410	12	Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.	0	Note

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Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

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
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.14	Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	37	Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still	37 %	Note

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PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         1 Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
   1 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 27/03/2017; check.def file version of 24/03/2017

Datablock C8OBTBTOC8rtHB - ellipsoid plot