checkCIF/PLATON report

Structure factors have been supplied for datablock(s) re11

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: re11

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Bond precision:  C-C = 0.0070 A          Wavelength=0.81182

Cell:          a=12.695(3)        b=13.398(3)     c=16.971(3)
               alpha=103.75(3)    beta=99.65(3)   gamma=110.73(3)
Temperature:   100 K
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	Calculated	Reported
Volume	2519.6(13)	2519.5(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H40 B2 Fe N6 O22 S6	C38 H40 B2 Fe N6 O22 S6
Sum formula	C38 H40 B2 Fe N6 O22 S6	C38 H40 B2 Fe N6 O22 S6
Mr	1202.59	1202.59
Dx,g cm-3	1.585	1.585
Z	2	2
Mu (mm-1)	0.907	0.920
F000	1236.0	1236.0
F000’	1239.48	
h,k,lmax	16,17,21	16,16,21
Nref	10784	10618
Tmin,Tmax	0.847,0.955	0.754,0.905
Tmin’	0.832	

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Correction method= # Reported T Limits: Tmin=0.754 Tmax=0.905
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 31.010

R(reflections)= 0.0693( 8926)     wR2(reflections)= 0.1575( 10618)

S = 1.013                 Npar= 685
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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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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S2 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.007 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.319 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         96 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.02A   From O9             0.49 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From N4            -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22             -0.32 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      14.04 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.81182 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          2 Units
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)        0.03 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1      --N5        .        5.2 s.u.
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O1             112.1 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O2             112.1 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O3             112.3 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O4             111.3 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O5             110.7 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O6             112.1 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  S6       ..C6              3.29 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O9       ..C23             2.94 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O13      ..C5              2.93 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         67 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         46 Note
PLAT984_ALERT_1_G The Fe-f'=       0.368 Deviates from the B&C-Value      0.356   Ch
PLAT984_ALERT_1_G The  O-f'=       0.016 Deviates from the B&C-Value      0.015   Ch
PLAT984_ALERT_1_G The  S-f'=       0.152 Deviates from the B&C-Value      0.154   Ch
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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
20 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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 30/01/2018; check.def file version of 30/01/2018

Datablock re11 - ellipsoid plot