checkCIF/PLATON report

Structure factors have been supplied for datablock(s) g170918a

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: g170918a

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Bond precision:   C-C = 0.0123 A          Wavelength=0.71073

Cell:             a=12.4749(10)     b=15.2567(15)      c=30.993(3)
                  alpha=90          beta=91.788(7)     gamma=90
Temperature:      295 K
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	Calculated	Reported
Volume	5895.9(9)	5895.9(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C64 H39 Br4 Cl Fe N4 O2 [+ solvent]	C64 H39 Br4 Cl Fe N4 O2
Sum formula	C64 H39 Br4 Cl Fe N4 O2 [+ solvent]	C64 H39 Br4 Cl Fe N4 O2
Mr	1306.89	1306.93
Dx,g cm-3	1.472	1.472
Z	4	4
Mu (mm-1)	3.058	3.058
F000	2600.0	2600.0
F000'	2598.29	
h,k,lmax	14,18,36	14,18,36
Nref	10411	10396
Tmin,Tmax	0.485,0.737	0.562,1.000
Tmin'	0.461	

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Correction method= # Reported T Limits: Tmin=0.562 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.027
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R(reflections)= 0.0788(4872) wR2(reflections)= 0.2201(10396)

S = 0.989 Npar= 686

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 15 Note

Author Response: Beamstop theta-min limit set too high, large unit-cell etc

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Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
dull

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
blackish

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.137 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 47% Check
PLAT213_ALERT_2_C Atom Br3 has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C3 --C4 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C22 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C38 --C39 . 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C37 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C13 -C18 . 1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C35 -C40 . 1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01232 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.142 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

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Alert level G

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1 . 109.6 Degree
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) . 3.37 Info
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.5 Low
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
  1 ALERT level B = A potentially serious problem, consider carefully
 19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  7 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
  5 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 06/07/2023; check.def file version of 30/06/2023

Datablock g170918a - ellipsoid plot