checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0257_0m

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: mo_b0257_0m

Bond precision: C-C = 0.0161 A Wavelength=0.71073

Cell: a=16.1933(6) b=16.1933(6) c=15.5940(7)
alpha=90 beta=90 gamma=120
Temperature: 123 K

	Calculated	Reported
Volume	3541.3(4)	3541.3(3)
Space group	P 3 2 1	P 3 2 1
Hall group	P 3 2"	P 3 2"
Moiety formula	2(C63 H71 Br Fe3 N3 O6 Si4 Zn), Br4 Zn0.50 [+ solvent]	C63 H71 Br1 Fe3 N3 O6 Si4 Zn1, 0.5(Br4 Zn0.5)
Sum formula	C126 H142 Br6 Fe6 N6 O12 Si8 Zn2.50 [+ solvent]	C63 H71 Br3 Fe3 N3 O6 Si4 Zn1.25
Mr	3135.14	1567.58
Dx,g cm-3	1.470	1.470
Z	1	2
Mu (mm-1)	2.827	2.827
F000	1589.0	1589.0
F000'	1591.16	
h,k,lmax	22,22,21	22,22,21
Nref	6356[3499]	6334
Tmin,Tmax	0.113,0.202	0.008,0.045
Tmin'	0.085	

Correction method= # Reported T Limits: Tmin=0.008 Tmax=0.045
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00 Theta(max)= 29.083

R(reflections)= 0.0622(5684) wR2(reflections)= 0.1746(6334)

S = 1.064 Npar= 272

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

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

PLAT213_ALERT_2_A	Atom C22	has ADP max/min Ratio	13.1 prolat
PLAT213_ALERT_2_A	Atom C24	has ADP max/min Ratio	13.1 prolat

Alert level B

PLAT213_ALERT_2_B	Atom C8	has ADP max/min Ratio	4.1 prolat
PLAT220_ALERT_2_B	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	8.5 Ratio
PLAT234_ALERT_4_B	Large Hirshfeld Difference C8 -- C9	..	0.28 Ang.
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of		C8 Check
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds		0.01612 Ang.
PLAT919_ALERT_3_B	Reflection # Likely Affected by the Beamstop ...		1 Check
PLAT987_ALERT_1_B	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms ..		Please Check
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density		2.73 eA-3
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range		7.4 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Fe1 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.4 Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600		3 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		3 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1 Check
PLAT975_ALERT_2_C	Check Calcd Residual Density 0.78A From	O2	0.42 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H7	-0.36 eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0 Note

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		5 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		1 Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .		0.017 Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.50 Check
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size		0.82 mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		11.25 Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of <C20	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C21	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C22	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C23	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C24	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C25	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H21	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H22	is Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H23	is Constrained at	0.3333 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of <H24    is Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H25    is Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Br2    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Br3    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Zn2    is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          7 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..        100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.75) in Resd. #          2 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ...        123 A**3
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         11 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        19 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
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          9 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
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  3 ALERT level A = Most likely a serious problem - resolve or explain
  7 ALERT level B = A potentially serious problem, consider carefully
 12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 34 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
 27 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_EXPT005_mo_b0257_0m
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_PLAT213_mo_b0257_0m
;
PROBLEM: Atom C22             has ADP max/min Ratio .....       13.1 prolat
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 26/02/2017; check.def file version of 21/02/2017

Datablock mo_b0257_0m - ellipsoid plot