

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0163_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_b0163_0m

Bond precision: C-C = 0.0065 A

Wavelength=0.71073

Cell: a=13.3015(6) b=18.8578(8) c=26.1725(11)
 alpha=69.599(1) beta=87.491(1) gamma=83.102(2)
Temperature: 100 K

	Calculated	Reported
Volume	6108.7(5)	6108.7(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H68 Br2 Fe4 N2 O3 Si4 Zn, C3 H6 O, H2 O	2(C52 H68 Br2 Fe4 N2 O3 Si4 Zn), 2(C3 H6 O), 2(H2 O)
Sum formula	C55 H76 Br2 Fe4 N2 O5 Si4 Zn	C110 H152 Br4 Fe8 N4 O10 Si8 Zn2
Mr	1406.13	2812.25
Dx,g cm-3	1.529	1.529
Z	4	2
Mu (mm-1)	2.746	2.746
F000	2880.0	2880.0
F000'	2886.38	
h,k,lmax	17,24,34	17,24,34
Nref	29528	29463
Tmin,Tmax	0.484,0.798	0.569,0.998
Tmin'	0.474	

Correction method= # Reported T Limits: Tmin=0.569 Tmax=0.998
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 28.000

R(reflections)= 0.0473(24584)

wR2(reflections)= 0.1251(29463)

S = 1.022

Npar= 1344

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

PLAT213_ALERT_2_A	Atom C8	has ADP max/min Ratio	7.6	prolat
PLAT413_ALERT_2_A	Short Inter XH3 .. XHn	H91B .. H4LD	..	1.79	Ang.
PLAT417_ALERT_2_A	Short Inter D-H..H-D	H1WB .. H2WA	..	1.38	Ang.
PLAT971_ALERT_2_A	Check Calcd Residual Density	0.81Å From Fe7		4.32	eA-3

Alert level B

PLAT220_ALERT_2_B	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min) Range	7.2	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C7 -- C8	..	11.8	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C8 -- C9	..	11.2	s.u.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H1WB .. H2WB	..	1.94	Ang.
PLAT420_ALERT_2_B	D-H Without Acceptor	O1W -- H1WA	...		Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O2W -- H2WB	...		Please Check
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s)	Below Theta(Min)		17	Note
PLAT971_ALERT_2_B	Check Calcd Residual Density	1.21Å From Si8		3.44	eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density		3.48	eA-3	
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent		4	Check	
PLAT213_ALERT_2_C	Atom C7	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C24	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C26	has ADP max/min Ratio	4.0	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 2	C	Ueq(max)/Ueq(min) Range	5.1	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1	H	Uiso(max)/Uiso(min) Range	7.7	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 2	H	Uiso(max)/Uiso(min) Range	5.4	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C8	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Fe1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Si1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Si8	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C2L	Check	
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00645	Ang.	
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H50A .. H4LE	..	2.11	Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H91B .. H6LD	..	2.14	Ang.
PLAT415_ALERT_2_C	Short Inter D-H..H-X	H2WA .. H86	..	2.14	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of		52	Ang3	
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600	35	Report	
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)		1	Check	
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.75Å From Br4	2.11	eA-3	
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.93Å From C4LA	1.90	eA-3	
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.26Å From C1L	1.83	eA-3	
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.20Å From C1L	1.61	eA-3	
PLAT972_ALERT_2_C	Check Calcd Residual Density	0.64Å From Fe7	-2.15	eA-3	
PLAT972_ALERT_2_C	Check Calcd Residual Density	0.66Å From Br4	-1.73	eA-3	
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.49Å From O2W	-1.26	eA-3	
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.52Å From O2W	-1.14	eA-3	
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.74Å From O2W	-0.92	eA-3	
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.89Å From O1W	-0.76	eA-3	
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.95Å From O1W	-0.70	eA-3	
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H3LA	-0.34	eA-3	
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H4LE	-0.33	eA-3	

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	16	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	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
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	24.90	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)..	100	% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)..	100	% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (5.60) in Resd. #	3	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (4.40) in Resd. #	5	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C6LA	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C4LA	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for O1	133.6	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for O4	133.4	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	30	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C3 H6 O	4	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	7	Note
PLAT793_ALERT_4_G	The Model has Chirality at Si2 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si3 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si6 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si7 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	13	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	30	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Note

4 **ALERT level A** = Most likely a serious problem - resolve or explain
8 **ALERT level B** = A potentially serious problem, consider carefully
34 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
44 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
20 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.

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_PLAT213_mo_b0163_0m
;
PROBLEM: Atom C8                has ADP max/min Ratio .....    7.6 prolat
RESPONSE: ...
;
_vrf_PLAT413_mo_b0163_0m
;
PROBLEM: Short Inter XH3 .. XHn    H91B    ..  H4LD    ..    1.79 Ang.
RESPONSE: ...
;
_vrf_PLAT417_mo_b0163_0m
;
PROBLEM: Short Inter D-H..H-D      H1WB    ..  H2WA    ..    1.38 Ang.
RESPONSE: ...
;
_vrf_PLAT971_mo_b0163_0m
;
PROBLEM: Check Calcd Residual Density  0.81A From    Fe7    4.32 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

