

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) i

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: i

Bond precision:	C-C = 0.0071 A	Wavelength=0.71073
Cell:	a=5.6690 (4)	b=12.3300 (9) c=14.1339 (9)
	alpha=91.644 (6)	beta=96.314 (6) gamma=92.400 (6)
Temperature:	173 K	
	Calculated	Reported
Volume	980.54 (12)	980.54 (12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H8 N4 S, C6 F4 I2	C12 H8 N4 S, C6 F4 I2
Sum formula	C18 H8 F4 I2 N4 S	C18 H8 F4 I2 N4 S
Mr	642.14	642.14
Dx, g cm ⁻³	2.175	2.175
Z	2	2
Mu (mm ⁻¹)	3.363	3.363
F000	604.0	604.0
F000'	602.63	
h, k, lmax	7, 15, 18	7, 15, 18
Nref	4499	4439
Tmin, Tmax	0.702, 0.790	0.490, 0.790
Tmin'	0.258	

Correction method= # Reported T Limits: Tmin=0.490 Tmax=0.790
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 27.484

R(reflections)= 0.0333 (3662)	wR2(reflections)=
S = 1.043	0.0960 (4439)
Npar= 263	

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report
0 4 0, 0 -2 1, -1 -1 1, 1 1 1, 0 3 1, -1 4 1,
0 -2 2, 1 1 2, 0 2 2, -2 3 2, -1 -2 3, 1 -1 3,
0 -2 4, -1 0 4, -2 1 4, 0 3 4, -1 2 5, 2 -2 6,
6 -2 6, 3 3 13, 2 3 15,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 14 Note
0 4 0, -1 -1 1, 1 1 1, -1 4 1, 0 -2 2, 1 1 2,
-2 3 2, -1 -2 3, 1 -1 3, 0 -2 4, -2 1 4, 0 3 4,
-1 2 5, 2 -2 6,

Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT431_ALERT_2_G Short Inter HL..A Contact I1 ..N1 . 2.80 Ang.
x,y,z = 1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact I2 ..N4 . 2.95 Ang.
-2+x,1+y,1+z = 1_366 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact I2 ..C10 . 3.45 Ang.
-2+x,1+y,1+z = 1_366 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C6 F4 I2
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
0 1 0, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 37 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1-1 3) Est.d BASF 0.25 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
0 1 0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.91 Note
Predicted wR2: Based on SigI**2 3.30 or SHELX Weight 9.49

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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