

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zfwang8_173k

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: zfwang8_173k

Bond precision:	C-C = 0.0056 A	Wavelength=1.54184
Cell:	a=13.71879 (14)	b=12.33193 (13) c=10.59252 (11)
	alpha=90	beta=90 gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	1792.03 (3)	1792.03 (3)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C16 H16 I O2 S, B F4	C16 H16 I O2 S, B F4
Sum formula	C16 H16 B F4 I O2 S	C16 H16 B F4 I O2 S
Mr	486.06	486.06
Dx, g cm ⁻³	1.802	1.802
Z	4	4
Mu (mm ⁻¹)	15.571	15.571
F000	952.0	952.0
F000'	955.22	
h, k, lmax	16, 15, 13	16, 15, 12
Nref	3558 [1880]	3298
Tmin, Tmax	0.452, 0.536	0.489, 1.000
Tmin'	0.342	

Correction method= # Reported T Limits: Tmin=0.489 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.93 Theta (max)= 72.427

R(reflections)= 0.0180 (3255)	wR2(reflections)= 0.0435 (3298)
S = 1.076	Npar= 228

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

PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	0.0011	Check
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check



Alert level G

PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		B1	Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1 ..01 .		2.77	Ang.
	1/2+x,1/2-y,z =	4_555		Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C11 .		3.01	Ang.
	-1/2+x,1/2-y,z =	4_455		Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..F2 .		2.96	Ang.
	x,y,z =	1_555		Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..F4 .		3.26	Ang.
	x,y,z =	1_555		Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		8	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	Info

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
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

