

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tboae

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: tboae

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=9.5657(3) b=10.2949(3) c=11.3068(3)
 alpha=87.3159(10) beta=77.1684(8) gamma=67.3284(10)
Temperature: 296 K

	Calculated	Reported
Volume	1000.84(5)	1000.85(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C17 H15 N O5 S), C7 H6 N O2	2(C17 H15 N O5 S), C7 H6 N O2
Sum formula	C41 H36 N3 O12 S2	C41 H36 N3 O12 S2
Mr	826.85	826.85
Dx,g cm-3	1.372	1.372
Z	1	1
Mu (mm-1)	0.201	0.201
F000	431.0	431.0
F000'	431.47	
h,k,lmax	11,12,13	11,12,13
Nref	3875	3865
Tmin,Tmax	0.960,0.988	0.959,0.988
Tmin'	0.959	

Correction method= MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.850

R(reflections)= 0.0373(2629)

wR2(reflections)= 0.1141(3865)

S = 1.073

Npar= 308

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

PLAT234_ALERT_4_C	Large Hirshfeld Difference C1	--	C5B	..	0.21 Ang.
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for			C1 Check
PLAT420_ALERT_2_C	D-H Without Acceptor	*N2	-	*H2A	... Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	*N2	-	*H2B	... Please Check
PLAT910_ALERT_3_C	Missing # of FCF Reflections Below Th(Min)			8 Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600			2 Report

● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms			5 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range	Identical			? Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	Sb	--	C4	.. 17.5 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C1	--	C5A	.. 9.2 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O7	--	C24	.. 7.0 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	N2	--	C20	.. 15.8 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C20	--	C21	.. 17.2 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C23	--	C24_a	.. 15.6 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C24	--	C23_a	.. 15.6 su
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =		24 Note
PLAT335_ALERT_2_G	Check Large C6 Ring	C-C Range C20	-C20_a		0.32 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels			2 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL				2014 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 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
3 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*, 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.

