

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) psu-1671lea-219-2

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: psu-1671lea-219-2

Bond precision:	C-C = 0.0087 A	Wavelength=0.71073	
Cell:	a=46.539 (16)	b=15.327 (5)	c=13.430 (3)
	alpha=90	beta=90	gamma=90
Temperature:	295 K		
	Calculated	Reported	
Volume	9580 (5)	9579 (5)	
Space group	F d d 2	F d d 2	
Hall group	F 2 -2d	F 2 -2d	
Moiety formula	C28 H19 N3 O4 S	C28 H19 N3 O4 S	
Sum formula	C28 H19 N3 O4 S	C28 H19 N3 O4 S	
Mr	493.52	493.52	
Dx, g cm ⁻³	1.369	1.369	
Z	16	16	
Mu (mm ⁻¹)	0.176	0.176	
F000	4096.0	4096.0	
F000'	4099.77		
h, k, lmax		63, 21, 18	
Nref		4615	
Tmin, Tmax	0.974, 0.993	0.632, 1.000	
Tmin'	0.974		

Correction method= # Reported T Limits: Tmin=0.632 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= Theta (max)= 29.455

R(reflections)= 0.0597 (2624)	wR2(reflections)=
S = 1.030	0.1422 (4615)
Npar= 330	

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

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00868 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 34 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 7.605 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.664 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
22 12 6, 28 14 6, 23 11 7, 29 13 7, 28 12 8, 30 12 8,
31 11 9,



Alert level G

PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C15 . 3.00 Ang.
x,-1/2+y,1/2+z = 5_545 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
4 0 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 445 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage 51 %
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

0 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
7 ALERT type 3 Indicator that the structure quality may be low
1 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.

