

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) psu-387da-enhyd

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-387da-enhyd

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Bond precision:    C-C = 0.0024 Å

Wavelength=0.71073

Cell:                a=11.0448(11)        b=12.2377(13)        c=13.2136(13)  
                      alpha=99.391(9)    beta=104.791(9)    gamma=103.693(9)  
Temperature:    295 K

	Calculated	Reported
Volume	1629.5(3)	1629.5(3)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C39 H31 N3 O5	C39 H31 N3 O5
Sum formula	C39 H31 N3 O5	C39 H31 N3 O5
Mr	621.67	621.67
Dx,g cm-3	1.267	1.267
Z	2	2
Mu (mm-1)	0.085	0.085
F000	652.0	652.0
F000'	652.30	
h,k,lmax	15,16,18	14,15,16
Nref	8963	7531
Tmin,Tmax	0.965,0.979	0.838,1.000
Tmin'	0.958	

Correction method= # Reported T Limits: Tmin=0.838 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.840

Theta(max)= 29.360

R(reflections)= 0.0526( 5408)

wR2(reflections)= 0.1468( 7531)

S = 1.069

Npar= 430

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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

PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....	7.018	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min)	8	Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	3	Report



### Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF		Please Do !
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.009	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle from 120 Deg for O4	107.0	Degree
PLAT793_ALERT_4_G	The Model has Chirality at C1 (Centro SPGR)		R Verify
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1197	Note
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ	2	Units
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 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  
3 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.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock psu-387da-enhyd - ellipsoid plot

