checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cj1506

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: Cj1506

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Bond precision:  C-C = 0.0029 A          Wavelength=1.54184

Cell:          a=10.7538(1)      b=15.3298(2)     c=15.9068(2)
               alpha=85.368(1)   beta=74.027(1)   gamma=84.442(1)
Temperature:   123 K
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	Calculated	Reported
Volume	2505.18(5)	2505.18(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C29 H43 N O	?
Sum formula	C29 H43 N O	C29 H43 N O
Mr	421.64	421.64
Dx,g cm-3	1.118	1.118
Z	4	4
Mu (mm-1)	0.497	0.497
F000	928.0	928.0
F000’	930.30	
h,k,lmax	12,18,19	12,18,19
Nref	9124	9104
Tmin,Tmax	0.831,0.933	0.804,1.000
Tmin’	0.804	

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Correction method= # Reported T Limits: Tmin=0.804 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 67.995

R(reflections)= 0.0745( 7966)     wR2(reflections)= 0.2185( 9104)

S = 1.047                 Npar= 588
```

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.11 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.74 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --C30 . 5.3 s.u.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.937 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82A From O1 0.61 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C44 --C45 . 5.8 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 19% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H43 ..H45A . 1.94 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H51 ..H46C . 2.05 Ang.
x,y,z = 1_555 Check
PLAT411_ALERT_2_G Short Inter H...H Contact H54A ..H48C . 2.00 Ang.
2-x,1-y,1-z = 2_766 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 13 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 80% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

3 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
6 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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 13/07/2021; check.def file version of 13/07/2021

Datablock Cj1506 - ellipsoid plot