

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0053 Å

Wavelength=0.71073

Cell: a=11.1004(9) b=11.3611(8) c=13.2166(9)
 alpha=65.350(3) beta=89.871(4) gamma=81.713(3)
Temperature: 293 K

	Calculated	Reported
Volume	1495.97(19)	1495.97(19)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C14 H19 N O5	C14 H19 N O5
Sum formula	C14 H19 N O5	C14 H19 N O5
Mr	281.30	281.30
Dx,g cm-3	1.249	1.249
Z	4	4
Mu (mm-1)	0.095	0.095
F000	600.0	600.0
F000'	600.34	
h,k,lmax	12,12,14	12,12,14
Nref	4061	3976
Tmin,Tmax	0.977,0.977	0.977,0.977
Tmin'	0.977	

Correction method= # Reported T Limits: Tmin=0.977 Tmax=0.977
AbsCorr = MULTI-SCAN

Data completeness= 0.979

Theta(max)= 22.780

R(reflections)= 0.0576(2685)

wR2(reflections)= 0.1650(3976)

S = 1.040

Npar= 402

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 A

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.5448$

**Author Response: Resolution in endo-3b is lower than expected, however,
the data were of sufficient quality to determine the connectivity.**

PLAT023_ALERT_3_A Resolution (too) Low [$\sin(\theta)/\lambda < 0.6$].. 0.54 Ang-1

**Author Response: Resolution in endo-3b is lower than expected, however,
the data were of sufficient quality to determine the connectivity.**

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 12 Note

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.89 Note
PLAT199_ALERT_1_C Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_C Reported _diffrn_ambient_temperature (K) 293 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00527 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.545 71 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for C23 --C24A . 8.6 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 10% Note
PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 5% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H15 ..H23D . 2.11 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H15 ..H23A . 2.13 Ang.
x,y,z = 1_555 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 7 Check
C9A -O3 -C9B 1.555 1.555 1.555 34.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 134 Check
C24B -C23 -H23B 1.555 1.555 1.555 17.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 137 Check
C24A -C23 -H23C 1.555 1.555 1.555 17.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 145 Check
H23A -C23 -H23D 1.555 1.555 1.555 2.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 148 Check
C23 -C24A -H23C 1.555 1.555 1.555 37.30 Deg.
PLAT793_ALERT_4_G Model has Chirality at C1 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C3 (Centro SPGR) S Verify

PLAT793_ALERT_4_G Model has Chirality at C6	(Centro SPGR)	R Verify
PLAT793_ALERT_4_G Model has Chirality at C15	(Centro SPGR)	S Verify
PLAT793_ALERT_4_G Model has Chirality at C17	(Centro SPGR)	S Verify
PLAT793_ALERT_4_G Model has Chirality at C20	(Centro SPGR)	R Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters		1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		38 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/		2018 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still		38% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by		6 Check

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

1 **ALERT level A** = Data missing that is essential or data in wrong format
 1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

