

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BAB8

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: BAB8

Bond precision: C-C = 0.0034 A Wavelength=0.71073

Cell: a=21.4765(8) b=21.4765(8) c=14.3538(6)
 alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	6620.6(6)	6620.5(4)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C19 H14 N4 O2	C19 H14 N4 O2
Sum formula	C19 H14 N4 O2	C19 H14 N4 O2
Mr	330.34	330.34
Dx,g cm-3	1.326	1.326
Z	16	16
Mu (mm-1)	0.090	0.090
F000	2752.0	2752.0
F000'	2753.11	
h,k,lmax	26,26,17	26,26,17
Nref	3324	3290
Tmin,Tmax	0.987,0.990	0.691,0.746
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.691 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 26.200

R(reflections)= 0.0482(2034) wR2(reflections)= 0.1567(3290)

S = 1.017 Npar= 227

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

PLAT430_ALERT_2_C	Short Inter D...A Contact	O1	..	O1	..	2.86	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min)					7	Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600				31	Report

● Alert level G

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
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...					2 Units
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O2	..	C1	..	2.96 Ang.
PLAT793_ALERT_4_G	The Model has Chirality at C9			(Centro SPGR)		R Verify
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.					2 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
6 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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 24/11/2016; check.def file version of 23/11/2016

Datablock BAB8 - ellipsoid plot

