

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: g-auto

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=29.045(4) b=8.2636(10) c=7.7063(8)
 alpha=90 beta=96.624(6) gamma=90

Temperature: 273 K

	Calculated	Reported
Volume	1837.3(4)	1837.3(4)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C16 H20 Ca N2 O8	?
Sum formula	C16 H20 Ca N2 O8	C16 H20 Ca N2 O8
Mr	408.42	408.42
Dx,g cm-3	1.477	1.476
Z	4	4
Mu (mm-1)	0.389	0.389
F000	856.0	856.0
F000'	857.39	
h,k,lmax	38,11,10	38,11,10
Nref	2294	2292
Tmin,Tmax		0.666,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.999 Theta(max)= 28.340

R(reflections)= 0.0516(2087) wR2(reflections)= 0.1557(2292)

S = 1.104 Npar= 129

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

PLAT420_ALERT_2_B D-H Without Acceptor O4 --H4 . Please Check

🟢 Alert level C

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O4 --C2 . 5.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 --C1 . 5.3 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cal Check

🟣 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 273 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.35 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints 2 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

- 0 **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
9 **ALERT level G** = General information/check it is not something unexpected

- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
2 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

