**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](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

**Datablock: I**

Bond precision: C-C = 0.0320 A Wavelength=0.71073

Cell: a=18.778(5) b=12.079(3) c=25.052(9)

alpha=90 beta=106.402(5) gamma=90

Temperature: 120 K

Calculated Reported Volume 5451(3) 5451(3) Space group C 2/c C 1 2/c 1

Hall group -C 2yc -C 2yc

Moiety formula C40 H42 Ba3 O32, 4(H2 O) C40 H42 Ba3 O32, 4(H2 O) Sum formula C40 H50 Ba3 O36 C40 H50 Ba3 O36

Mr 1518.79 1518.82

Dx,g cm-3 1.851 1.851

Z 4 4

Mu (mm-1) 2.246 2.246

F000 2984.0 2984.0

F000’ 2981.96

h,k,lmax 22,14,29 22,14,29

Nref 4804 4798

Tmin,Tmax 0.973,0.978 0.005,0.024

Tmin’ 0.956

Correction method= # Reported T Limits: Tmin=0.005 Tmax=0.024

AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 24.998

R(reflections)= 0.1254( 4200) wR2(reflections)= 0.2955( 4798) S = 1.223 Npar= 378

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**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 1.42A From O16 -3.73 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT976\_ALERT\_2\_A Check Calcd Resid. Dens. 0.61A From O16’ -3.21 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

**Alert level B**

PLAT342\_ALERT\_3\_B Low Bond Precision on C-C Bonds ............... 0.032 Ang.

**Author Response: The best available crystal was still very small and, therefore, of low reflective power.**

PLAT971\_ALERT\_2\_B Check Calcd Resid. Dens. 1.22A From Ba1 2.82 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT971\_ALERT\_2\_B Check Calcd Resid. Dens. 0.90A From Ba2 2.67 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_B Check Calcd Resid. Dens. 0.61A From O16’ -3.21 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_B Check Calcd Resid. Dens. 0.94A From Ba1 -2.73 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT977\_ALERT\_2\_B Check Negative Difference Density on H16B -1.99 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

**Alert level C**

[PLAT018\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/PLAT018.html) \_diffrn\_measured\_fraction\_theta\_max .NE. \*\_full ! Check [PLAT082\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT082.html) High R1 Value .................................. 0.13 Report [PLAT084\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT084.html) High wR2 Value (i.e. > 0.25) ................... 0.30 Report [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C18 --C19 . 0.24 Ang. [PLAT314\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT314.html) Small Angle for H2O: Metal-O16’ -H16B . 87.30 Degree [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 19.693 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 3.478 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 2.028 Check [PLAT911\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT911.html) Missing FCF Refl Between Thmin & STh/L= 0.595 7 Report [PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.22A From Ba1 2.28 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.39A From O15 2.12 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.47A From O16’ 1.84 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.23A From O16 1.79 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.44A From O16’ 1.61 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.53A From O16’ -2.43 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.14A From O8 -2.31 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.37A From O8 -2.28 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.84A From Ba2 -1.94 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.73A From Ba2 -1.70 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.98A From O16’ 1.14 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.88A From O12 0.93 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.10A From O11 0.88 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.99A From O16 -1.28 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 1.09A From O3 -1.27 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H5 -0.56 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H11 -0.86 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H13A -0.36 eA-3

**Author Response: This probably arises from strong absorption effects that were not fully corrected for.**

**Alert level G**

[PLAT002\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT002.html) Number of Distance or Angle Restraints on AtSite 5 Note [PLAT003\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT003.html) Number of Uiso or Uij Restrained non-H Atoms ... 7 Report [PLAT004\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT004.html) Polymeric Structure Found with Maximum Dimension 1 Info

[PLAT007\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT007.html) Number of Unrefined Donor-H Atoms .............. 17 Report [PLAT083\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT083.html) SHELXL Second Parameter in WGHT Unusually Large 686.71 Why ? [PLAT171\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT171.html) The CIF-Embedded .res File Contains EADP Records 6 Report [PLAT172\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT172.html) The CIF-Embedded .res File Contains DFIX Records 1 Report [PLAT176\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT176.html) The CIF-Embedded .res File Contains SADI Records 1 Report [PLAT186\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT186.html) The CIF-Embedded .res File Contains ISOR Records 3 Report [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O13 Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O13’ Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O15 Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O15’ Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O16 Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of O16’ Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H15A Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H15B Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H15C Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H15D Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H16A Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H16B Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H16C Constrained at 0.5 Check [PLAT300\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT300.html) Atom Site Occupancy of H16D Constrained at 0.5 Check [PLAT301\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT301.html) Main Residue Disorder ..............(Resd 1 ) 13% Note [PLAT302\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT302.html) Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note [PLAT309\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT309.html) Single Bonded Oxygen (C-O > 1.3 Ang) ........... O2 Check [PLAT398\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT398.html) Deviating C-O-C Angle From 120 for O12 105.5 Degree [PLAT416\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT416.html) Short Intra D-H..H-D H14B ..H16B . 1.85 Ang.

-x,y,1/2-z = 2\_555 Check

[PLAT417\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H16B ..H17A . 1.73 Ang. x,y,z = 1\_555 Check

[PLAT722\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT722.html) Angle Calc 129.00, Rep 127.80 Dev... 1.20 Degree

H16C -O16 -H16D 1.555 1.555 1.555 # 232 Check [PLAT860\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT860.html) Number of Least-Squares Restraints ............. 44 Note [PLAT909\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT909.html) Percentage of I>2sig(I) Data at Theta(Max) Still 71% Note [PLAT941\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT941.html) Average HKL Measurement Multiplicity ........... 3.3 Low [PLAT978\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT978.html) Number C-C Bonds with Positive Residual Density. 0 Info

2 **ALERT level A** = Most likely a serious problem - resolve or explain

6 **ALERT level B** = A potentially serious problem, consider carefully

27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

34 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

35 ALERT type 2 Indicator that the structure model may be wrong or deficient

10 ALERT type 3 Indicator that the structure quality may be low

20 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](http://journals.iucr.org/services/cif/checking/checkform.html) 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 05/12/2020; check.def file version of 05/12/2020**

**Datablock** ·**ellipsoid plot**

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NOMOVE FORCED Prob

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