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: 15_20srv262

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Bond precision:   C-C = 0.0048 A          Wavelength=0.71073

Cell:             a=13.1637(2)      b=13.1637(2)      c=15.4431(4)
                  alpha=90          beta=90           gamma=120
Temperature:      120 K

                 Calculated                Reported
Volume           2317.51(9)                2317.51(9)
Space group      P 32                      P 32
Hall group       P 32                      P 32
Moiety formula   C44 H34                   C44 H34
Sum formula      C44 H34                   C44 H34
Mr               562.71                    562.71
Dx,g cm-3        1.210                     1.210
Z                3                         3
Mu (mm-1)        0.068                     0.068
F000             894.0                     894.0
F000'            894.32
h,k,lmax         17,17,21                  17,17,21
Nref             8204[ 4102]               8165
Tmin,Tmax        0.987,0.995               0.686,0.746
Tmin'            0.978

Correction method= # Reported T Limits: Tmin=0.686 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.99/1.00        Theta(max)= 28.983

R(reflections)= 0.0542( 7144)                wR2(reflections)=
                                             0.1217( 8165)
S = 1.032                 Npar= 404
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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

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 0.61 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
STRVA01_ALERT_4_C Flack test results are meaningless.
From the CIF: _refine_ls_abs_structure_Flack -0.100
From the CIF: _refine_ls_abs_structure_Flack_su 1.000
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00482 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C18 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18A Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18C Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17C Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17D Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18D Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18E Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18F Constrained at 0.3 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 2% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H9 ..H18B . 2.03 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C31 ..C18A 3.13 Ang.
2-y,2+x-y,-1/3+z = 2_774 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 2 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 58.0 Degree

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

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

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  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
 16 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 18/12/2021; check.def file version of 18/12/2021

Datablock 15_20srv262 - ellipsoid plot