checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cj1504

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: Cj1504

Bond precision: C-C = 0.0042 A Wavelength=1.54184

Cell: a=11.8341(10) b=16.6685(19) c=18.3950(15)
alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	3628.5(6)	3628.5(6)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C41 H59 K N2	?
Sum formula	C41 H59 K N2	C41 H59 K N2
Mr	619.00	619.00
Dx,g cm-3	1.133	1.133
Z	4	4
Mu (mm-1)	1.485	1.485
F000	1352.0	1352.0
F000’	1356.59	
h,k,lmax	14,20,22	14,20,22
Nref	3501	3489
Tmin,Tmax	0.948,0.956	0.832,1.000
Tmin’	0.849	

Correction method= # Reported T Limits: Tmin=0.832 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 68.993

R(reflections)= 0.0638(2663) wR2(reflections)= 0.1731(3489)

S = 1.100 Npar= 328

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

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00423 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.670 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         4 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         6 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C2       --C3B      .       8.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C12        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18C       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21C       Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        52% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C10      - C11      .       1.52 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C17      - C18      .       1.52 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C20      - C21      .       1.52 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        20 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        16 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        30 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         5 Info
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 40 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 26 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 13/07/2021; check.def file version of 13/07/2021

Datablock Cj1504 - ellipsoid plot