

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0136 Å

Wavelength=0.71073

Cell: a=8.300(1) b=16.191(2) c=21.221(3)
 alpha=108.167(4) beta=94.071(5) gamma=104.453(4)
Temperature: 100 K

	Calculated	Reported
Volume	2589.3(6)	2589.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H20 N4, 2(I3), I2	?
Sum formula	C11 H20 I8 N4	C22 H40 I16 N8
Mr	1223.51	2447.02
Dx,g cm-3	3.139	3.138
Z	4	2
Mu (mm-1)	9.587	9.586
F000	2152.0	2152.0
F000'	2137.75	
h,k,lmax	9,19,25	9,19,25
Nref	9458	9410
Tmin,Tmax	0.115,0.563	0.377,0.747
Tmin'	0.049	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 25.350

R(reflections)= 0.0377(8865)

wR2(reflections)= 0.1083(9410)

S = 1.018

Npar= 415



PLAT434_ALERT_2_A Short Inter HL..HL Contact I3 ..I12 3.25 Ang.
x,y,z = 1_555 Check

Author Response: these are long intramolecular distances featuring the I5-polyiodide or short I...I secondary bonds. All these distances are discussed in the manuser



PLAT434_ALERT_2_B Short Inter HL..HL Contact I4 ..I13 3.39 Ang.
1-x,1-y,-z = 2 665 Check

Author Response: these are long intramolecular distances featuring the I5-polyiodide or short I...I secondary bonds. All these distances are discussed in the manuscript

PLAT434_ALERT_2_B Short Inter HL..HL Contact I5 ..I16 3.40 Ang.
x,y,z = 1 555 Check

Author Response: these are long intramolecular distances featuring the I5-polyiodide or short I...I secondary bonds. All these distances are discussed in the manuscript



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DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -4.595
Test value = -3.975
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -4.59 eA-3
PLAT213_ALERT_2_C Atom C11 has ADP max/min Ratio ..... 3.5 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N4 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01362 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N3 --H3A . Please Check
PLAT420_ALERT_2_C D-H Without Acceptor N7 --H7A . Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C11 H20 N4

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PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	10	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT	Unusually Large	27.23 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records		1 Report
PLAT434_ALERT_2_G Short Inter HL..HL Contact I8	..I14	3.59 Ang.
	1+x,y,z =	1_655 Check

Author Response: these are long intramolecular distances featuring the I5-polyiodide or short I...I secondary bonds. All these distances are discussed in the manuscript

PLAT434_ALERT_2_G Short Inter HL..HL Contact I10	..I11	3.52 Ang.
	-x,1-y,-z =	2_565 Check

Author Response: these are long intramolecular distances featuring the I5-polyiodide or short I...I secondary bonds. All these distances are discussed in the manuscript

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2 Note
C11 H20 N4	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	4 Note
I3	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	7 Note
I2	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	9 Note
I2	
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters	1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	18 Note

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

 - 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 15 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
 - 7 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.

