

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Zh361

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: Zh361

Bond precision:	C-C = 0.0091 Å	Wavelength=0.71073
Cell:	a=11.4609(12)	b=18.020(2) c=19.186(3)
	alpha=112.896(7)	beta=100.698(8) gamma=101.699(5)
Temperature:	296 K	
	Calculated	Reported
Volume	3417.3(8)	3417.2(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C8 H21 B12 N2, C16 H36 N	?
Sum formula	C24 H57 B12 N3	C24 H57 B12 N3
Mr	517.45	517.44
Dx,g cm-3	1.006	1.006
Z	4	4
Mu (mm-1)	0.053	0.053
F000	1128.0	1128.0
F000'	1128.23	
h,k,lmax	14,23,24	14,23,24
Nref	15690	15532
Tmin,Tmax	0.981,0.998	
Tmin'	0.979	

Correction method= Not given

Data completeness= 0.990 Theta(max)= 27.498

R(reflections)= 0.0891(4265) wR2(reflections)= 0.2784(15532)

S = 0.903 Npar= 769

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**

PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 27% Check

Author Response: Small crystal.

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 57 Note

Author Response: Closed by beamstop.

**Alert level B**

PLAT234_ALERT_4_B Large Hirshfeld Difference C12 --C13 . 0.27 Ang.
 PLAT234_ALERT_4_B Large Hirshfeld Difference C13 --C14 . 0.28 Ang.

**Alert level C**

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report
 PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
 C54A
 PLAT221_ALERT_2_C Solv./Anion Resd 3 C Ueq(max)/Ueq(min) Range 4.4 Ratio
 PLAT223_ALERT_4_C Solv./Anion Resd 3 H Ueq(max)/Ueq(min) Range 5.5 Ratio
 PLAT223_ALERT_4_C Solv./Anion Resd 4 H Ueq(max)/Ueq(min) Range 4.6 Ratio
 PLAT230_ALERT_2_C Hirshfeld Test Diff for C33 --C34 . 6.6 s.u.
 PLAT230_ALERT_2_C Hirshfeld Test Diff for C63 --C64 . 5.6 s.u.
 PLAT234_ALERT_4_C Large Hirshfeld Difference C32 --C33 . 0.17 Ang.
 PLAT234_ALERT_4_C Large Hirshfeld Difference C41 --C42 . 0.16 Ang.
 PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C83 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3A Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C31 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C52 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C61 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C63 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C71 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C73 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C82 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including N3 0.145 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including N4 0.108 Check
 PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C3 --C8 . 1.37 Ang.
 PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C3A --C8A . 1.37 Ang.
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00906 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C13 - C14 . 1.42 Ang.
 PLAT420_ALERT_2_C D-H Without Acceptor N1 --H1B . Please Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 14.314 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.401 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 27 Report

**Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 22 Note
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
 PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
 PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
 PLAT300_ALERT_4_G Atom Site Occupancy of C23A Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of C23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C44A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C44B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44F	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		24%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		12%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H21A ..H24F .		2.13 Ang.	
	x,y,z =	1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H41A ..H44E .		2.14 Ang.	
	x,y,z =	1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H51A ..H54F .		2.00 Ang.	
	x,y,z =	1_555	Check	
PLAT414_ALERT_2_G	Short Intra D-H..H-X H2C ..H5A		2.10 Ang.	
	x,y,z =	1_555	Check	
PLAT415_ALERT_2_G	Short Inter D-H..H-X H1C ..H4 .		2.07 Ang.	
	x,y,z =	1_555	Check	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		8	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		55	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		76	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 29 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
 41 ALERT type 4 Improvement, methodology, query or suggestion
 1 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 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.

