

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) RGFBS32701

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: RGFBS32701

Bond precision: C-C = 0.0039 Å Wavelength=0.71073

Cell: a=16.9634 (4) b=16.9634 (4) c=9.8413 (3)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2831.90 (16)	2831.90 (15)
Space group	P -4 21 c	P -4 21 c
Hall group	P -4 2n	P -4 2n
Moiety formula	C13 H20 N2, C2 H3 N	C15 H23 N3
Sum formula	C15 H23 N3	C15 H23 N3
Mr	245.36	245.36
Dx, g cm ⁻³	1.151	1.151
Z	8	8
Mu (mm ⁻¹)	0.069	0.069
F000	1072.0	1072.0
F000'	1072.31	
h, k, lmax	20, 20, 12	20, 20, 12
Nref	2788 [1578]	2783
Tmin, Tmax	0.987, 0.990	0.702, 0.745
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.76/1.00 Theta (max)= 25.999

R(reflections)= 0.0427 (2662)

wR2(reflections)=
0.1195 (2783)

S = 1.146

Npar= 204

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**

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: `_refine_ls_abs_structure_Flack` 0.500
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.500
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C13 H20 N2
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

● **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.500 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0010 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0010 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 2.75 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H5 ..H15A . 1.68 Ang.
 $-1/2+x, -3/2-y, 1/2-z =$ 6_435 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H6 ..H15C . 1.65 Ang.
 $1+y, -x, 1-z =$ 3_656 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H8 ..H15B . 1.84 Ang.
 $x, y, z =$ 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H10B ..H15E . 1.92 Ang.
 $3/2-x, -1/2+y, 1/2-z =$ 5_645 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H12A ..H15F . 1.86 Ang.
 $1+y, -x, -z =$ 3_655 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X H8 ..H2 . 2.10 Ang.
 $x, y, z =$ 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N1 ..C15B . 2.81 Ang.
 $3/2-x, -1/2+y, 1/2-z =$ 5_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N2 ..C15 . 2.86 Ang.
 $x, y, z =$ 1_555 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C2 H3 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
C2 H3 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints 56 Note
PLAT883_ALERT_1_G No Info/Value for `_atom_sites_solution_primary` . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.10 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 4 Note

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
12 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 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.

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