

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) multi

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: multi

Bond precision: N- B = 0.0020 Å Wavelength=1.54178

Cell: a=10.1552(2) b=10.1654(3) c=11.0614(2)
 alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1141.89(5)	1141.89(5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C7 H21 B N P	?
Sum formula	C7 H21 B N P	C7 H21 B N P
Mr	161.03	161.03
Dx, g cm ⁻³	0.937	0.937
Z	4	4
Mu (mm ⁻¹)	1.660	1.660
F000	360.0	360.0
F000'	361.80	
h, k, lmax	12, 12, 13	12, 12, 13
Nref	1076	1074
Tmin, Tmax	0.764, 0.904	0.848, 1.000
Tmin'	0.534	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 67.044

R(reflections)= 0.0344(831) wR2(reflections)= 0.1087(1074)

S = 1.014 Npar= 110

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

Crystal system given = orthorhombic

PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 0.9367 Check

🟢 Alert level C

PLAT019_ALERT_1_C _diffrn_measured_fraction_theta_full/_max < 1.0 0.990 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.76 Note
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for N1 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C7 H21 B N P
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.597 2 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 1 Note

🟠 Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds 6 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C1 -- C3A .. 5.4 su
PLAT301_ALERT_3_G Main Residue Disorder Percentage = 50 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 15 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.35 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C1 -- C2B . 1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C1 -- C2B . 1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2A -- C4A . 1.97 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4A -- C2A . 1.97 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3B -- C4B . 1.88 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4B -- C3B . 1.88 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 5 Check
C1 -P1 -C4B 1.555 1.555 7.565 42.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 13 Check
P1 -B1 -P1 1.555 1.555 7.565 24.27 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 20 Check
C3B -C1 -C3B 7.565 1.555 1.555 39.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 31 Check
C2A -C1 -C2A 1.555 1.555 7.565 32.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 32 Check
C4A -C1 -C3A 7.565 1.555 1.555 24.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 37 Check
C4A -C1 -C3A 1.555 1.555 7.565 24.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 44 Check
C4B -C1 -C2B 1.555 1.555 7.565 41.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 47 Check
C4B -C1 -C2B 7.565 1.555 1.555 41.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 52 Check
C1 -C2A -C4A 1.555 1.555 7.565 43.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 85 Check
C3A -C4A -H4AC 7.565 1.555 1.555 43.60 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 18 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 58 %

0 ALERT level A = Most likely a serious problem - resolve or explain

1 ALERT level B = A potentially serious problem, consider carefully

6 ALERT level C = Check. Ensure it is not caused by an omission or oversight

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

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

9 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
14 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*, 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.

