

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0061 A	Wavelength=0.71073
Cell:	a=7.8725(4)	b=10.9122(6) c=15.6053(8)
	alpha=103.034(2)	beta=96.915(2) gamma=92.460(2)
Temperature:	100 K	
	Calculated	Reported
Volume	1293.15(12)	1293.15(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 H4 Br4 N2	C10 H4 Br4 N2
Sum formula	C10 H4 Br4 N2	C10 H4 Br4 N2
Mr	471.75	471.79
Dx, g cm ⁻³	2.423	2.423
Z	4	4
Mu (mm ⁻¹)	12.421	12.421
F000	872.0	872.0
F000'	868.25	
h, k, lmax	11, 15, 21	11, 15, 21
Nref	7543	7528
Tmin, Tmax	0.063, 0.155	0.101, 0.747
Tmin'	0.006	

Correction method= # Reported T Limits: Tmin=0.101 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 29.999

R(reflections)= 0.0417(6176)	wR2(reflections)= 0.1069(7528)
S = 1.038	Npar= 289

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00606 Ang.



Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT431_ALERT_2_G Short Inter HL..A Contact Br2B ..N4A . 3.09 Ang.
1+x,-1+y,z = 1_645 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Br8A ..N10B . 3.16 Ang.
1-x,1-y,1-z = 2_666 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Br12 ..N4B . 3.15 Ang.
-x,1-y,2-z = 2_567 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br13 ..C5A . 3.33 Ang.
x,-1+y,z = 1_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C11B ..C11B . 3.17 Ang.
1-x,-y,1-z = 2_656 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br6A ..Br6B . 3.46 Ang.
x,y,z = 1_555 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 11 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 60.0 Degree

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 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.

