

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: shelxl

Bond precision: C-C = 0.0087 A Wavelength=0.71075

Cell: a=11.969(3) b=11.969(3) c=14.415(4)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2065.1(12)	2065.0(12)
Space group	P 43 21 2	P 43 21 2
Hall group	P 4nw 2abw	P 4nw 2abw
Moiety formula	C9 H10 N3, Br	0.5(C36 H40 N12), 2(Br)
Sum formula	C9 H10 Br N3	C18 H20 Br2 N6
Mr	240.10	480.22
Dx,g cm-3	1.544	1.545
Z	8	4
Mu (mm-1)	3.939	3.939
F000	960.0	960.0
F000'	958.02	
h,k,lmax	14,14,17	14,14,17
Nref	1819[1103]	1814
Tmin,Tmax	0.351,0.473	0.367,0.472
Tmin'	0.319	

Correction method= NUMERICAL

Data completeness= 1.64/1.00 Theta(max)= 24.993

R(reflections)= 0.0282(1544) wR2(reflections)= 0.0642(1814)

S = 0.975 Npar= 119

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

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 9.27 Note
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0087 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Dimension 1 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero -0.034
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by 2.00 Ratio
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
Br

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
2 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*, 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.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

