

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5

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: 5

Bond precision: C-C = 0.0126 Å Wavelength=0.71073

Cell: a=6.9692(3) b=9.2930(4) c=21.4788(10)
 alpha=97.000(4) beta=97.013(4) gamma=110.805(4)
Temperature: 173 K

	Calculated	Reported
Volume	1270.00(11)	1269.99(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H8 Br2 O3	C14 H8 Br2 O3
Sum formula	C14 H8 Br2 O3	C14 H8 Br2 O3
Mr	384.00	384.02
Dx, g cm ⁻³	2.008	2.008
Z	4	4
Mu (mm ⁻¹)	6.382	6.382
F000	744.0	744.0
F000'	742.15	
h, k, lmax	9, 12, 29	9, 12, 29
Nref	7047	5822
Tmin, Tmax	0.569, 0.682	0.762, 1.000
Tmin'	0.557	

Correction method= # Reported T Limits: Tmin=0.762 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.826 Theta(max)= 29.467

R(reflections)= 0.0798(4246)	wR2(reflections)=
S = 1.323	0.1506(5822)
Npar= 343	

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

PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01264	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	17.617	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.889	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	35	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H12 .	-0.33	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H21 .	-0.33	eA-3



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.52	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6 .	109.6	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O26 .	109.9	Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1188	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

