

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1tbe

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: 1tbe

Bond precision: C-C = 0.0140 Å Wavelength=1.54184

Cell: a=7.2697(4) b=7.9781(4) c=9.4586(3)
 alpha=100.930(4) beta=104.580(4) gamma=110.313(5)
Temperature: 100 K

	Calculated	Reported
Volume	474.15(5)	474.14(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 H12 Br2 N4 Pt, C2 H2 Br4	C6 H12 Br2 N4 Pt, C2 H2 Br4
Sum formula	C8 H14 Br6 N4 Pt	C8 H14 Br6 N4 Pt
Mr	840.71	840.78
Dx, g cm ⁻³	2.944	2.945
Z	1	1
Mu (mm ⁻¹)	28.603	28.603
F000	378.0	378.0
F000'	369.80	
h,k,lmax	8,9,11	8,9,11
Nref	1816	1806
Tmin,Tmax	0.019,0.032	0.674,1.000
Tmin'	0.003	

Correction method= # Reported T Limits: Tmin=0.674 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 70.315

R(reflections)= 0.0409(1558) wR2(reflections)= 0.1135(1806)

S = 1.113 Npar= 90

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.9	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.014	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.84A From Pt1	-2.49	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.82A From Pt1	-1.90	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.00A From Pt1	-1.59	eA-3



Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pt1	--Br1	.	16.3	s.u.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Br1	..Br1S		3.37	Ang.
		x,y,z =	1_555	Check	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Br1	..Br2S		3.46	Ang.
		-1+x,-1+y,z =	1_445	Check	
PLAT794_ALERT_5_G	Tentative Bond Valency for Pt1	(II)	.	2.31	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600			6	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...			2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			2.2	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
8 **ALERT level G** = General information/check it is not something unexpected

0 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
3 ALERT type 3 Indicator that the structure quality may be low
1 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* 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.

