

Structure factors have been supplied for datablock(s) siv72

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0060 Å	Wavelength=0.71073
Cell:	a=12.5845 (9)	b=7.0519 (5) c=13.8263 (10)
	alpha=90	beta=113.098 (3) gamma=90
Temperature:	120 K	
	Calculated	Reported
Volume	1128.65 (14)	1128.65 (14)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C2 H9 B10 Cl3	C2 H9 B10 Cl3
Sum formula	C2 H9 B10 Cl3	C2 H9 B10 Cl3
Mr	247.54	247.54
Dx, g cm-3	1.457	1.457
Z	4	4
Mu (mm-1)	0.754	0.754
F000	488.0	488.0
F000'	489.81	
h, k, lmax	15, 8, 17	15, 8, 17
Nref	2220 [1112]	2197
Tmin, Tmax	0.986, 0.990	0.953, 0.990
Tmin'	0.985	

Data completeness= 1.98/0.99 Theta (max)= 26.027

R(reflections)= 0.0296(2116)	wR2(reflections)= 0.0700(2197)
S = 1.124	Npar= 178

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

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.25	Note
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.006	Ang.



Alert level G

PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	7%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C1 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C2 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C2 .	1.63	Ang.
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.8	Low
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units
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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
0 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.

