

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20230712_ys_bjsk_287_down_0

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: cu_20230712_ys_bjsk_287_down_0

Bond precision:	C-C = 0.0058 A	Wavelength=1.54178
Cell:	a=25.6161 (14)	b=25.6161 (14) c=16.3068 (13)
	alpha=90	beta=90 gamma=120
Temperature:	200 K	
	Calculated	Reported
Volume	9266.7 (13)	9266.7 (13)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C17 H22 N2 O2, C H2 Cl2 [+ solvent]	C H2 Cl2, C17 H22 N2 O2
Sum formula	C18 H24 Cl2 N2 O2 [+ solvent]	C18 H24 Cl2 N2 O2
Mr	371.29	371.29
Dx, g cm-3	1.198	1.198
Z	18	18
Mu (mm-1)	2.927	2.927
F000	3528.0	3528.0
F000'	3549.50	
h, k, lmax	30, 30, 19	30, 30, 19
Nref	3773	3752
Tmin, Tmax	0.697, 0.725	0.222, 0.320
Tmin'	0.632	

Correction method= # Reported T Limits: Tmin=0.222 Tmax=0.320

AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 68.396

R(reflections)= 0.0741(2146)

wR2(reflections)=
0.2383(3752)

S = 1.034

Npar= 220

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.47	Report
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C18	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11	0.126 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00582	Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.819	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	16 Report



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	465	A**3
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.2	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
5 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.

