

Structure factors have been supplied for datablock(s) Comopound-6h

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0044 Å	Wavelength=1.54184	
Cell:	a=7.282 (5)	b=14.476 (8)	c=12.212 (7)
	alpha=90	beta=103.047 (12)	gamma=90
Temperature:	293 K		

```
Correction method= # Reported T Limits: Tmin=0.718 Tmax=0.934
AbsCorr = MULTI-SCAN
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```
R(reflections)= 0.0871( 1436)      wR2(reflections)=
S = 0.966                          0.2828( 2296)
Npar= 173
```

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

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
 _refine_diff_density_min given = -0.620
 Test value = -0.600

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
 The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.65 eA-3

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.62 eA-3

PLAT199_ALERT_1_C Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_C Reported _diffrn_ambient_temperature (K) 293 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00438 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.744 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report

 2 0 0, 1 3 0, 1 4 0, 2 1 1, 2 2 1, 2 1 2,

 0 5 2, -2 2 3, 0 4 3, -1 2 4, 2 12 9, 3 9 10,

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 6 Check

PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 58.16 Check

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.08Ang From Ol . -0.43 eA-3

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report

 H1A H1B

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report

PLAT899_ALERT_4_G SHELXL-97 is Outdated and Succeeded by SHELXL 2019/3 Note

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

 1 0 0, 0 2 0, 0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note

 2 0 0, 1 3 0,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.346 Note

 Predicted wR2: Based on SigI**2 6.51 or SHELX Weight 29.29

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

