

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dtth5

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: dtth5

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Bond precision:      C-C = 0.0085 Å      Wavelength=0.71073

Cell:                      a=8.3626 (3)      b=40.8701 (18)      c=9.6924 (4)  
                                    alpha=90      beta=90      gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	3312.7 (2)	3312.7 (2)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C40 H24 O4 S3	?
Sum formula	C40 H24 O4 S3	C40 H24 O4 S3
Mr	664.77	664.77
Dx, g cm <sup>-3</sup>	1.333	1.333
Z	4	4
Mu (mm <sup>-1</sup> )	0.266	0.266
F000	1376.0	1376.0
F000'	1378.05	
h, k, lmax	10, 50, 11	10, 50, 11
Nref	3306	3200
Tmin, Tmax	0.938, 0.995	0.702, 0.746
Tmin'	0.923	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.968      Theta (max)= 26.013

R(reflections)= 0.1583 ( 2305)

wR2(reflections)=  
0.1964 ( 3200)

S = 1.589

Npar= 305

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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.

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**Alert level B**

PLAT082\_ALERT\_2\_B High R1 Value ..... 0.16 Report

**Author Response: Crystal quality was marginal and so is the data quality.  
The refinement statistics reflect this.**

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**Alert level C**

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00846 Ang.  
PLAT601\_ALERT\_2\_C Unit Cell Contains Solvent Accessible VOIDS of . 33 Ang\*\*3  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 124.120 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.378 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 15.547 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.417 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 6.025 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.264 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.945 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.076 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 47 Report  
10 0 0, 10 1 0, 10 2 0, 10 3 0, 10 4 0, 8 22 0,  
8 26 0, 8 28 0, 8 29 0, 9 7 1, 9 8 1, 9 21 1,  
8 23 1, 8 25 1, 8 28 1, 8 29 1, 9 11 2, 9 13 2,  
9 16 2, 9 18 2, 8 22 2, 8 26 2, 7 34 2, 9 4 3,  
9 7 3, 9 12 3, 9 14 3, 9 17 3, 8 20 3, 8 21 3,  
5 40 3, 9 0 4, 9 10 4, 9 11 4, 8 13 4, 9 13 4,  
7 30 4, 8 16 5, 8 8 6, 8 15 6, 7 23 6, 3 37 6,  
0 42 6, 6 0 8, 7 1 8, 5 15 9, 3 26 9,

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 21 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H Atoms 34 Report  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 9.02 Why ?  
PLAT175\_ALERT\_4\_G The CIF-Embedded .res File Contains SAME Records 2 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 1 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0200 Report  
PLAT189\_ALERT\_3\_G A Non-default SAME Restraint Value for First Par 0.0100 Report  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1) 43% Note  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C4 - C5 . 1.42 Ang.  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C6 - C7 . 1.44 Ang.  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 688 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note  
0 2 0, 0 4 0, 0 1 1,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 56 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 7 Note  
10 9 1, 10 8 1, 10 7 2, 9 11 2, 9 13 2, 9 4 3,  
9 7 3,  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 9.738 Note  
Predicted wR2: Based on SigI\*\*2 2.01 or SHELX Weight 12.37  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 2 Info

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

2 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  
15 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

