

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

Bond precision:	C-C = 0.0085 A	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 ⁻³	1.333	1.333
Z	4	4
Mu (mm ⁻¹)	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

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 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.**

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,

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

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

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.

