

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2

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: 1

Bond precision:	C-C = 0.0052 Å	Wavelength=0.71073
Cell:	a=8.0275(10)	b=7.8676(13) c=34.961(5)
	alpha=90	beta=90.106(9) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	2208.0(6)	2208.0(5)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H5 N3 O9, C6 H4 S4	C14 H5 N3 O9, C6 H4 S4
Sum formula	C20 H9 N3 O9 S4	C20 H9 N3 O9 S4
Mr	563.54	563.54
Dx,g cm-3	1.695	1.695
Z	4	4
Mu (mm-1)	0.492	0.492
F000	1144.0	1144.0
F000'	1146.56	
h,k,lmax	9,9,41	9,9,41
Nref	3908	3897
Tmin,Tmax	0.790,0.961	0.475,0.514
Tmin'	0.744	

Correction method= # Reported T Limits: Tmin=0.475 Tmax=0.514
AbsCorr = PSI-SCAN

Data completeness= 0.997 Theta(max)= 25.005

R(reflections)= 0.0490(2464) wR2(reflections)= 0.1458(3897)

S = 1.037 Npar= 326

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

PLAT019_ALERT_1_B	_diffn_measured_fraction_theta_full/_max < 1.0	0.975	Report
PLAT430_ALERT_2_B	Short Inter D...A Contact O16 .. O18 ..	2.84	Ang.

Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for O18 -- N17 ..	5.7	su
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0052	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact O15 .. O21 ..	2.88	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H8A .. S32 ..	3.02	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	2.806	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.595	11	Report

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max) still	31	%
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...	1	Report

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 2

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073	
Cell:	a=19.078(5)	b=7.2068(14)	c=19.443(4)
	alpha=90	beta=117.833(12)	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	2364.0(9)	2364.0(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C15 H7 N3 O9, C6 H4 S4	C15 H7 N3 O9, C6 H4 S4
Sum formula	C21 H11 N3 O9 S4	C21 H11 N3 O9 S4
Mr	577.57	577.57
Dx,g cm-3	1.623	1.623
Z	4	4
Mu (mm-1)	0.462	0.462
F000	1176.0	1176.0
F000'	1178.57	
h,k,lmax	22,8,23	22,8,23
Nref	4181	4165
Tmin,Tmax	0.837,0.982	0.656,0.703
Tmin'	0.758	

Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.703
AbsCorr = PSI-SCAN

Data completeness= 0.996 Theta(max)= 25.022

R(reflections)= 0.0482(2393) wR2(reflections)= 0.1161(4165)

S = 1.002 Npar= 336

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

PLAT019_ALERT_1_B _diffn_measured_fraction_theta_full/_max < 1.0 0.977 Report



Alert level C

PLAT241_ALERT_2_C High	Ueq as Compared to Neighbors for	S30 Check
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	N21 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds		0.0052 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H14A .. O19 ..		2.65 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance		7.702 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595		15 Report



Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 1 Report

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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*, 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.

PLATON version of 29/01/2015; check.def file version of 29/01/2015



