

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) v18190_h

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: v18190_h

Bond precision:	C-C = 0.0056 A	Wavelength=1.54178
Cell:	a=12.4227(7)	b=10.3715(6) c=15.5943(9)
	alpha=90	beta=93.088(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	2006.3(2)	2006.3(2)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	2(C24 H28 O7), H2 O	2(C24 H28 O7), H2 O
Sum formula	C48 H58 O15	C48 H58 O15
Mr	874.94	874.94
Dx, g cm-3	1.448	1.448
Z	2	2
Mu (mm-1)	0.889	0.889
F000	932.0	932.0
F000'	935.11	
h, k, lmax	15, 13, 19	15, 13, 19
Nref	8676[4583]	8046
Tmin, Tmax	0.928, 0.948	0.660, 0.744
Tmin'	0.923	

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.744
AbsCorr = MULTI-SCAN

Data completeness= 1.76/0.93 Theta(max)= 79.031

R(reflections)= 0.0611(7375) wR2(reflections)= 0.1597(8046)

S = 1.064 Npar= 580

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

PLAT035_ALERT_1_B	_chemical_absolute_configuration	Info	Not Given	Please Do !
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density		0.83 eA-3	
PLAT420_ALERT_2_B	D-H Without Acceptor	06A	--H6A	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	08	--H8A	Please Check

🟡 Alert level C

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

PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00563 Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H14B ..H17C	2.02 Ang.
	-x,1/2+y,2-z =	2_557 Check
PLAT415_ALERT_2_C	Short Inter D-H..H-X H3AB ..H8A	2.13 Ang.
	-x,1/2+y,1-z =	2_556 Check
PLAT415_ALERT_2_C	Short Inter D-H..H-X H8A ..H17A	2.09 Ang.
	x,y,z =	1_555 Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D H1B ..H8B	2.11 Ang.
	x,y,z =	1_555 Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1 Note
	C24 H28 O7	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600 58 Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	88 %
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.83A From 05A	0.70 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.04A From 08	-0.46 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H8A	-0.44 eA-3

🟡 Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.10 Report
PLAT169_ALERT_4_G	The CIF-Embedded .res File Contains AFIX 1 Recds	2 Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 03A	102.2 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 04A	106.0 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 05A	107.1 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 03B	103.0 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 04B	105.9 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 05B	107.6 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C24 H28 O7	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3 Note
	H2 O	
PLAT791_ALERT_4_G	Model has Chirality at C1A	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C1B	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C2A	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C2B	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C4A	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C4B	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C5A	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C5B	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C6A	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C6B	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C9A	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C9B	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C10A	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C10B	(Chiral SPGR) R Verify
PLAT791_ALERT_4_G	Model has Chirality at C11A	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C11B	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C12A	(Chiral SPGR) S Verify
PLAT791_ALERT_4_G	Model has Chirality at C12B	(Chiral SPGR) S Verify

PLAT791_ALERT_4_G Model has Chirality at C13A	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C13B	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C15A	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C15B	(Chiral SPGR)	S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		84 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		5 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 28 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

