

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) v18645_a

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: v18645_a

Bond precision:	C-C = 0.0034 Å	Wavelength=1.54178	
Cell:	a=11.6776(5)	b=8.9076(4)	c=14.9231(7)
	alpha=90	beta=108.474(2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1472.30(12)	1472.30(12)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C34 H40 O6	C34 H40 O6	
Sum formula	C34 H40 O6	C34 H40 O6	
Mr	544.66	544.66	
Dx, g cm ⁻³	1.229	1.229	
Z	2	2	
Mu (mm ⁻¹)	0.667	0.667	
F000	584.0	584.0	
F000'	585.76		
h, k, lmax	14, 11, 19	14, 11, 19	
Nref	6468[3446]	5545	
Tmin, Tmax	0.923, 0.987	0.551, 0.754	
Tmin'	0.797		

Correction method= # Reported T Limits: Tmin=0.551 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 1.61/0.86 Theta(max)= 80.960

R(reflections)= 0.0353(5277) wR2(reflections)= 0.0895(5545)

S = 1.061 Npar= 367

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

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	value Low	.	0.944	Why?
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C5	--C14	.	12.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C5	--C20	.	15.5 s.u.

Alert level G

PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero	.	0.210	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 02		108.2	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 03		107.0	Degree
PLAT791_ALERT_4_G	Model has Chirality at C1	(Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C2	(Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C6	(Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C9	(Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C10	(Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C11	(Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C17	(Chiral SPGR)	S	Verify

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock v18645_a - ellipsoid plot

