

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) baran727_sq

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: baran727_sq

Bond precision: C-C = 0.0020 Å Wavelength=1.54178

Cell: a=15.6402(8) b=27.8107(15) c=7.0298(4)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	3057.7(3)	3057.7(3)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	C29 H46 O3 [+ solvent]	C29 H46 O3
Sum formula	C29 H46 O3 [+ solvent]	C29 H46 O3
Mr	442.66	442.66
Dx, g cm ⁻³	0.962	0.962
Z	4	4
Mu (mm ⁻¹)	0.464	0.464
F000	976.0	976.0
F000'	978.58	
h, k, lmax	19, 33, 8	19, 33, 8
Nref	5832[3335]	5820
Tmin, Tmax	0.911, 0.911	0.666, 0.753
Tmin'	0.911	

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.75/1.00 Theta(max)= 70.292

R(reflections)= 0.0280(5732) wR2(reflections)= 0.0752(5820)

S = 1.043 Npar= 298

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 G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT791_ALERT_4_G	Model has Chirality at C2 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C5 (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 C11 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C15 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C19 (Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C22 (Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C24 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C28 (Chiral SPGR)	R	Verify
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	21	Info

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

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

PLATON version of 17/03/2019; check.def file version of 04/03/2019

Datablock baran727_sq - ellipsoid plot

